Full wwPDB X-ray Structure Validation Report (i)

Nov 11, 2023 – 05:01 pm GMT

PDB ID	:	2C3O
Title	:	CRYSTAL STRUCTURE OF THE FREE RADICAL INTERMEDIATE OF PYRUVATE:FERREDOXIN OXIDOREDUCTASE FROM Desulfovibrio africanus
Authors	:	Cavazza, C.; Contreras-Martel, C.; Pieulle, L.; Chabriere, E.; Hatchikian, E.C.; Fontecilla-Camps, J.C.
Deposited on	:	2005-10-11
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

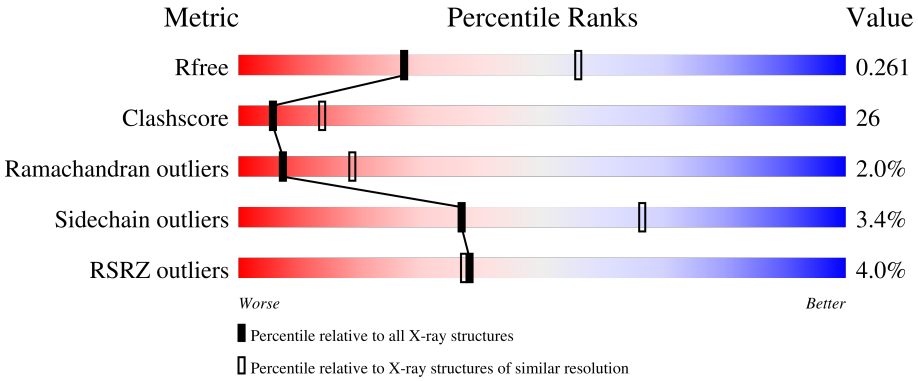
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1231	5% 56% 41% .
1	B	1231	3% 57% 40% .

2 Entry composition (i)

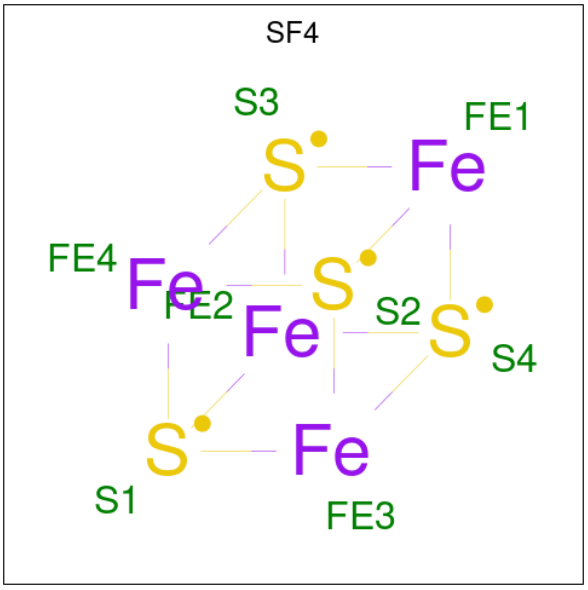
There are 7 unique types of molecules in this entry. The entry contains 19451 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PYRUVATE-FERREDOXIN OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			
1	B	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Fe	S		0	0
			8	4	4			
2	A	1	Total	Fe	S		0	0
			8	4	4			
2	A	1	Total	Fe	S		0	0
			8	4	4			
2	B	1	Total	Fe	S		0	0
			8	4	4			

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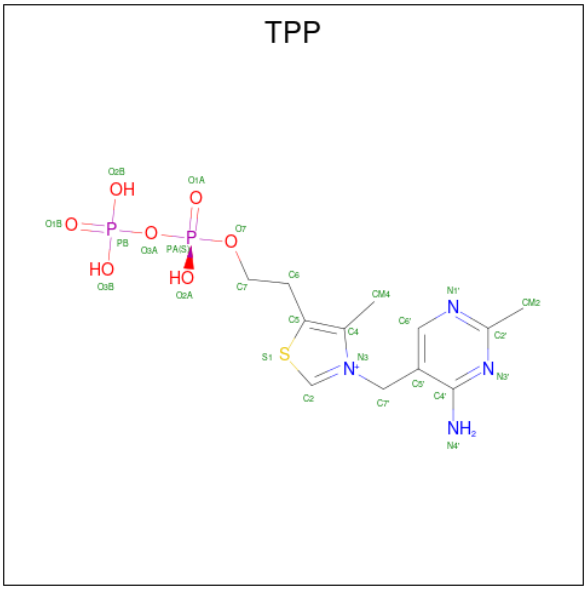
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 26 12 4 7 2 1	0	0
3	B	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0

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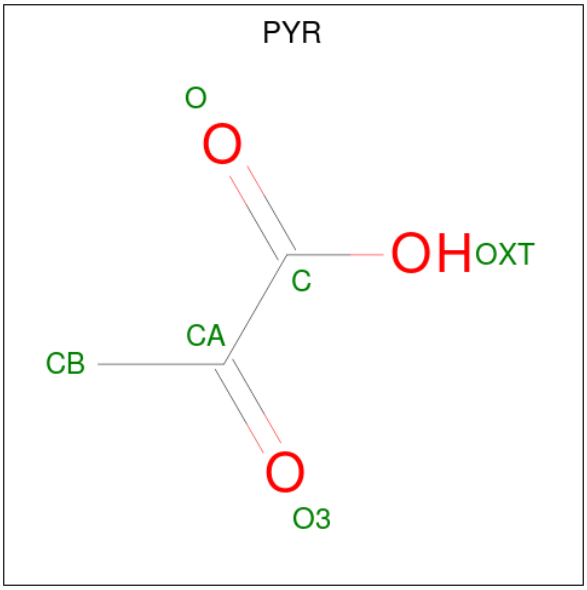
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

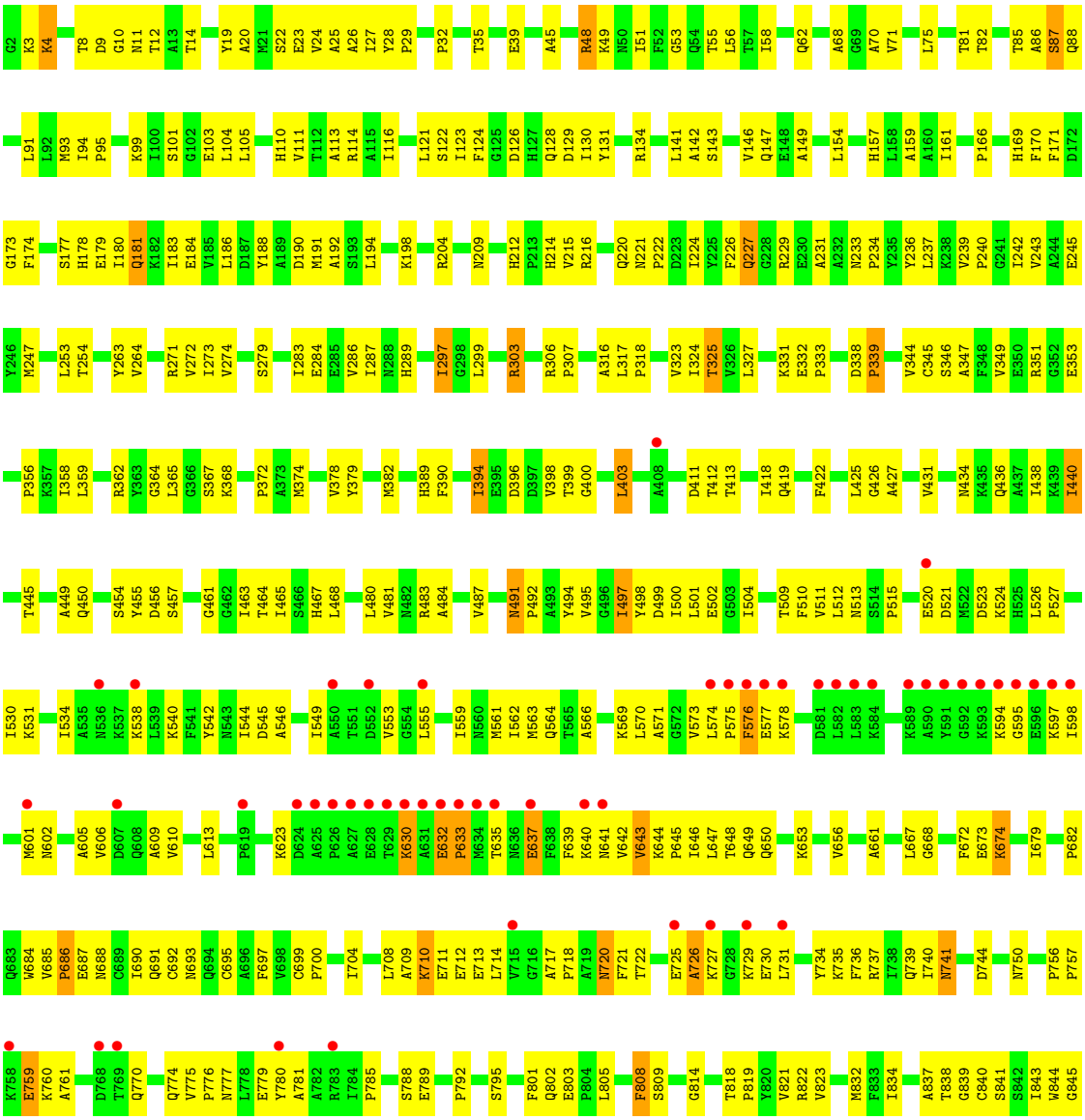
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	262	Total O 262 262	0	0
7	B	307	Total O 307 307	0	0

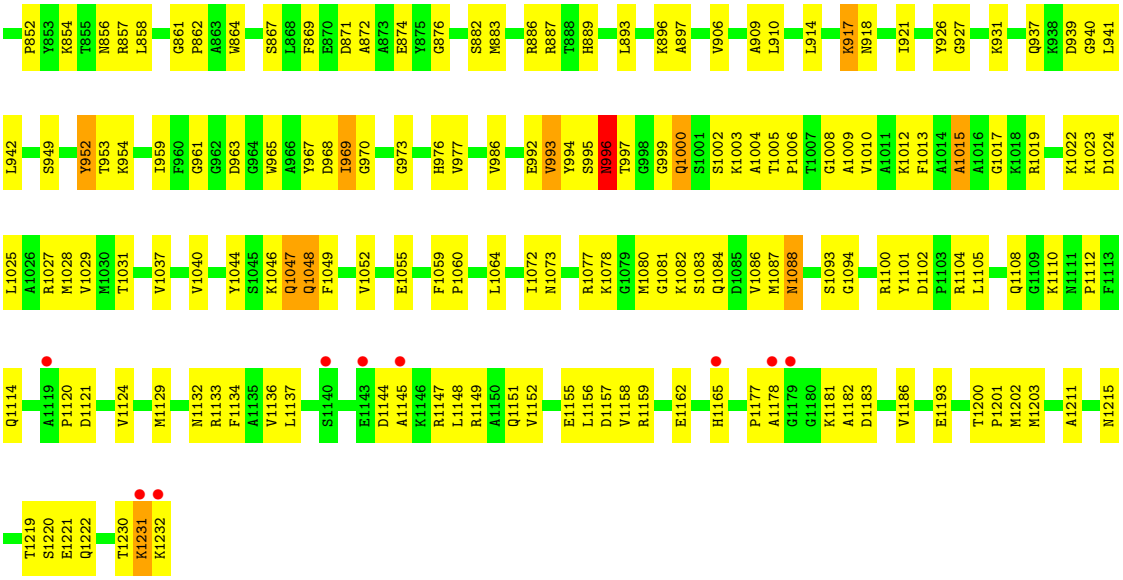
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

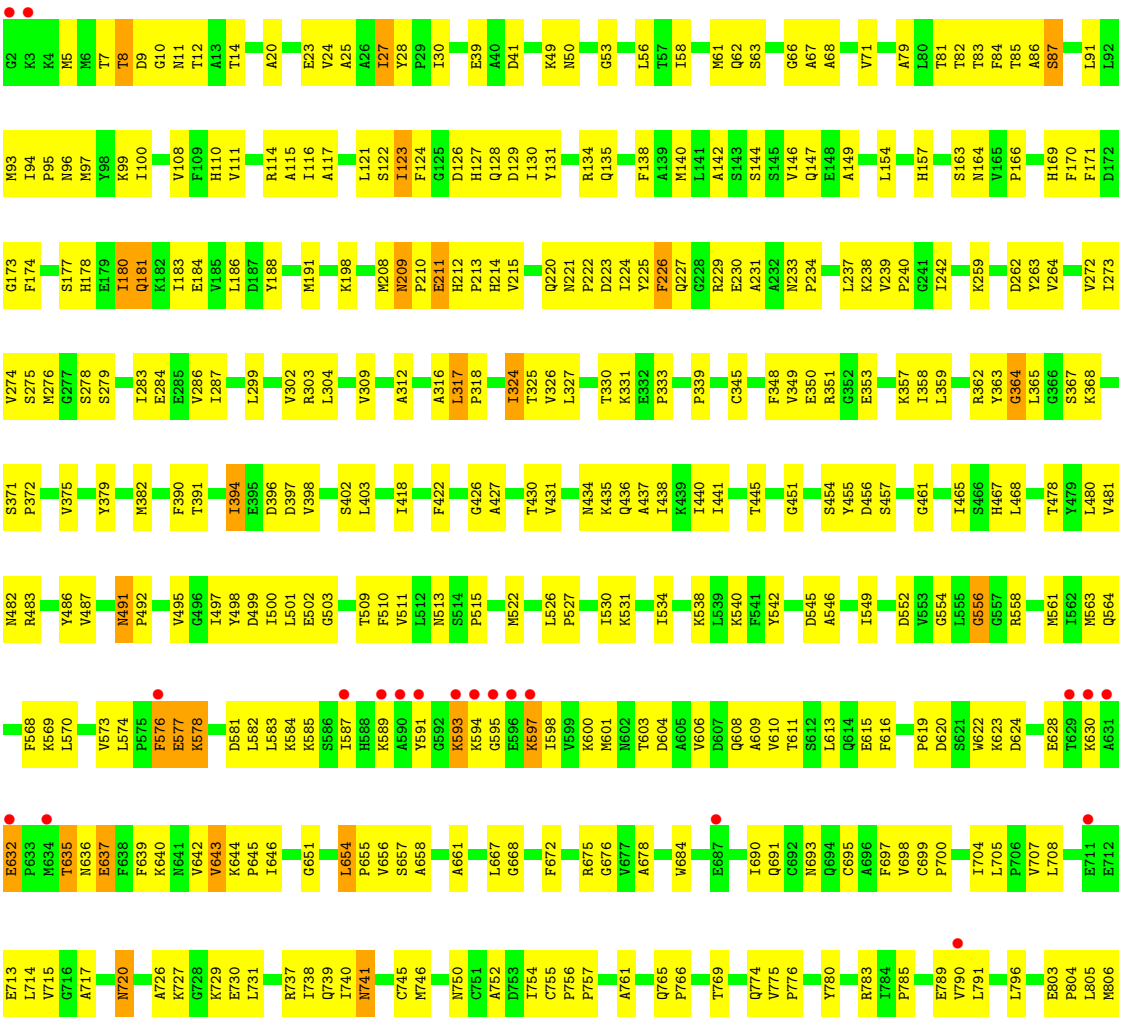
Chain A:

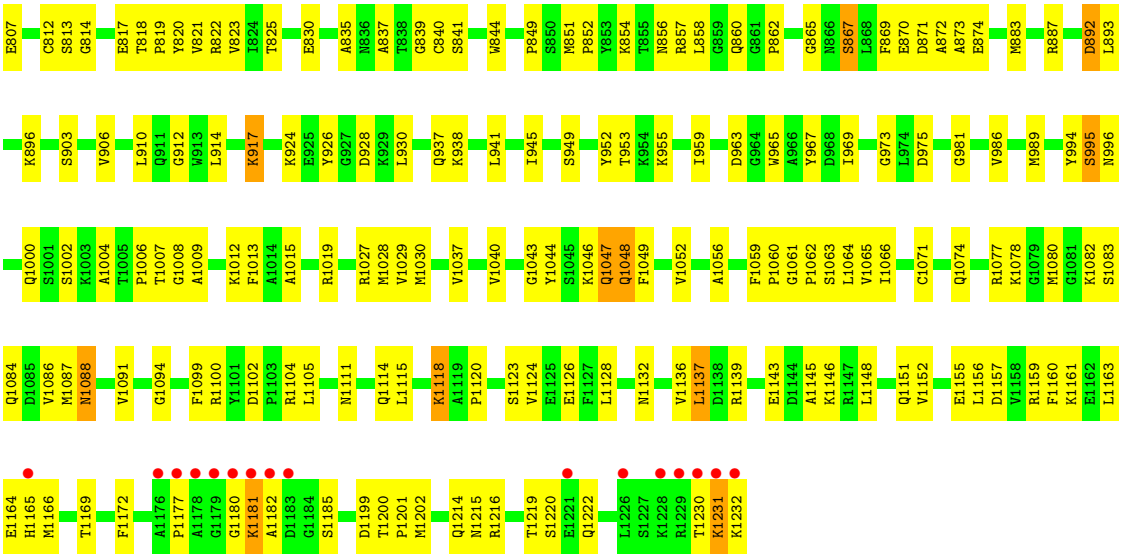




• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

Chain B:




E807 C812 S813 G814 E817 T818 P819 Y820 V821 R822 V823 I824 T825 E830 A835 N836 A837 T838 G839 C840 S841 W844 P849 S850 M851 P852 Y853 K854 T855 N856 R857 L858 G859 Q860 G861 P862 G865 N866 S867 L868 F869 E870 D871 A872 A873 E874 M883 R887 D892 L893
K896 S903 V906 L910 Q911 G912 W913 L914 K917 K924 E925 Y926 G927 D928 K929 L930 Q937 K938 L941 I945 S949 Y952 T953 K954 K955 I959 D963 G964 W965 A966 Y967 D968 I969 G973 L974 D975 G981 V986 M989 Y994 S995 N996
Q1000 S1001 S1002 K1003 A1004 T1005 P1006 T1007 G1008 A1009 K1012 F1013 A1014 A1015 R1019 R1027 M1028 V1029 M1030 V1037 V1040 G1043 Y1044 S1045 K1046 Q1047 Q1048 F1049 V1052 A1056 F1059 P1060 G1061 P1062 S1063 L1064 V1065 I1066 C1071 Q1074 R1077 K1078 G1079 M1080 G1081 K1082 S1083
Q1084 D1085 V1086 M1087 N1088 V1091 G1094 F1099 R1100 Y1101 D1102 P1103 R1104 L1105 N1111 Q1114 L1115 K1118 A1119 P1120 S1123 V1124 E1125 E1126 F1127 L1128 N1132 V1136 L1137 D1138 R1139 E1143 D1144 A1145 K1146 R1147 L1148 Q1151 V1152 E1155 L1156 D1157 V1158 R1159 F1160 K1161 E1162 L1163
E1164 H1165 M1166 T1169 F1172 A1176 P1177 A1178 G1179 G1180 K1181 A1182 D1183 G1184 S1185 D1199 T1200 P1201 M1202 Q1214 N1215 R1216 T1219 S1220 E1221 Q1222 L1226 S1227 K1228 R1229 T1230 K1231 K1232

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.65Å 145.24Å 204.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.11 – 2.70 38.11 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (38.11-2.70) 94.5 (38.11-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.268 0.197 , 0.261	Depositor DCC
R_{free} test set	3476 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19451	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, CA, SF4, MG, TPP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/9585	0.52	0/12954
1	B	0.29	0/9585	0.54	0/12954
All	All	0.29	0/19170	0.53	0/25908

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9383	0	9263	525	0
1	B	9383	0	9262	500	0
2	A	24	0	0	0	0
2	B	24	0	0	1	0
3	A	26	0	16	3	0
3	B	26	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	6	0	0	0	0
7	A	262	0	0	13	0
7	B	307	0	0	13	0
All	All	19451	0	18557	958	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (958) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:THR:HG22	1:A:1202:MET:H	1.19	1.06
1:B:1077:ARG:HH11	1:B:1077:ARG:HB2	1.22	1.02
1:B:239:VAL:HG13	1:B:240:PRO:HD3	1.42	1.02
1:A:198:LYS:H	1:A:198:LYS:HD2	1.24	1.00
1:A:147:GLN:HE22	1:A:184:GLU:H	1.10	0.97
1:A:690:ILE:HD11	1:A:692:CYS:HB3	1.44	0.97
1:A:1019:ARG:HH12	1:B:1180:GLY:HA3	1.27	0.96
1:B:198:LYS:H	1:B:198:LYS:HD2	1.28	0.96
1:B:1077:ARG:HB2	1:B:1077:ARG:NH1	1.81	0.94
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.50	0.94
1:B:12:THR:HG22	1:B:39:GLU:OE1	1.68	0.93
1:B:708:LEU:HD21	1:B:731:LEU:HD22	1.51	0.93
1:B:1200:THR:HG22	1:B:1202:MET:H	1.35	0.91
1:B:1102:ASP:OD1	1:B:1104:ARG:HG2	1.72	0.90
1:A:1080:MET:H	1:B:1215:ASN:ND2	1.71	0.89
1:B:274:VAL:HG23	1:B:324:ILE:HD11	1.55	0.89
1:B:817:GLU:HB3	1:B:989:MET:HE2	1.55	0.88
1:B:914:LEU:HD13	1:B:917:LYS:HZ1	1.38	0.87
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.57	0.87
1:A:1215:ASN:ND2	1:B:1080:MET:H	1.72	0.87
1:B:639:PHE:HA	1:B:643:VAL:HG13	1.54	0.87
1:A:737:ARG:HH11	1:A:739:GLN:HE22	1.23	0.86
1:B:643:VAL:HB	1:B:849:PRO:HB2	1.55	0.86
1:A:726:ALA:HB1	1:A:731:LEU:HB3	1.57	0.85
1:A:455:TYR:HB2	1:B:1201:PRO:HG3	1.60	0.84
1:B:914:LEU:HA	1:B:917:LYS:HZ3	1.42	0.82
1:A:509:THR:HG22	1:A:540:LYS:HB2	1.61	0.81
1:B:1231:LYS:HG3	1:B:1232:LYS:H	1.45	0.81
1:B:454:SER:HB3	1:B:465:ILE:HG23	1.61	0.81
1:A:12:THR:HG22	1:A:39:GLU:OE2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HD21	1:A:254:THR:HG22	1.63	0.81
1:B:1006:PRO:HG2	1:B:1009:ALA:HB2	1.62	0.81
1:A:1077:ARG:HH11	1:A:1077:ARG:HB2	1.44	0.80
1:A:128:GLN:HE22	1:B:229:ARG:HE	1.29	0.80
1:B:823:VAL:HG21	1:B:1049:PHE:HE2	1.47	0.80
1:B:9:ASP:OD2	1:B:12:THR:HG23	1.82	0.80
1:A:194:LEU:HD21	1:A:253:LEU:HD11	1.64	0.79
1:A:325:THR:HG22	1:A:382:MET:SD	2.23	0.79
1:A:273:ILE:HD13	1:A:325:THR:HG23	1.65	0.79
1:B:1132:ASN:HD21	1:B:1139:ARG:HH12	1.28	0.79
1:B:239:VAL:CG1	1:B:240:PRO:HD3	2.14	0.78
1:A:11:ASN:ND2	1:A:177:SER:HB2	1.98	0.78
1:A:398:VAL:HG13	1:A:656:VAL:HG13	1.65	0.77
1:A:1231:LYS:HG3	1:A:1232:LYS:H	1.50	0.77
1:A:491:ASN:HD22	1:A:492:PRO:HD2	1.48	0.77
1:B:691:GLN:HE22	1:B:727:LYS:H	1.30	0.77
1:A:1093:SER:HB2	1:A:1124:VAL:HG22	1.68	0.76
1:A:147:GLN:NE2	1:A:184:GLU:H	1.84	0.76
1:A:1219:THR:HG22	1:A:1221:GLU:H	1.51	0.76
1:B:1047:GLN:NE2	1:B:1047:GLN:H	1.82	0.76
1:A:1219:THR:HB	1:A:1222:GLN:HG3	1.67	0.76
1:A:8:THR:HB	1:A:12:THR:OG1	1.87	0.75
1:A:867:SER:O	1:B:99:LYS:HE3	1.87	0.75
1:A:438:ILE:HD11	1:A:468:LEU:HD22	1.68	0.75
1:B:1219:THR:HB	1:B:1222:GLN:HG3	1.66	0.75
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.87	0.75
1:B:994:TYR:CE1	1:B:1002:SER:HB3	2.22	0.74
1:B:837:ALA:HB2	1:B:872:ALA:HB2	1.70	0.74
1:A:1077:ARG:HB2	1:A:1077:ARG:NH1	2.02	0.74
1:A:287:ILE:HD11	1:A:379:TYR:OH	1.88	0.74
1:A:809:SER:HB2	1:A:844:TRP:O	1.88	0.74
1:A:1019:ARG:NH1	1:B:1181:LYS:H	1.85	0.74
1:A:1145:ALA:HB1	1:A:1149:ARG:HH12	1.53	0.74
1:B:573:VAL:HG23	1:B:574:LEU:HG	1.70	0.74
1:B:578:LYS:HB3	7:B:2151:HOH:O	1.88	0.74
1:B:1083:SER:O	1:B:1087:MET:HG3	1.88	0.74
1:B:644:LYS:HB3	1:B:645:PRO:HD3	1.70	0.74
1:A:487:VAL:HG23	1:A:504:ILE:HD13	1.70	0.73
1:A:909:ALA:HA	1:A:926:TYR:HD2	1.53	0.73
1:A:1215:ASN:HD21	1:B:1080:MET:H	1.35	0.73
1:B:593:LYS:HD2	1:B:594:LYS:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:PHE:HA	1:A:643:VAL:HG22	1.69	0.73
1:B:893:LEU:HB3	1:B:945:ILE:HD11	1.70	0.73
1:B:1143:GLU:O	1:B:1146:LYS:HG2	1.88	0.73
1:B:438:ILE:HD11	1:B:468:LEU:HD22	1.71	0.72
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.89	0.72
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.71	0.72
1:B:7:THR:HB	1:B:180:ILE:HD11	1.69	0.72
1:B:430:THR:HG22	1:B:434:ASN:HD21	1.54	0.72
1:B:1132:ASN:ND2	1:B:1139:ARG:HH12	1.86	0.72
1:B:56:LEU:HD23	1:B:58:ILE:HD11	1.71	0.72
1:B:1007:THR:HB	1:B:1152:VAL:HG22	1.70	0.72
1:B:445:THR:HG21	1:B:574:LEU:HD21	1.72	0.72
1:B:914:LEU:HA	1:B:917:LYS:NZ	2.05	0.72
1:B:123:ILE:HD13	1:B:123:ILE:H	1.55	0.72
1:A:222:PRO:HD3	1:B:124:PHE:CE2	2.25	0.71
1:B:11:ASN:ND2	1:B:177:SER:HB2	2.05	0.71
1:B:121:LEU:HD23	1:B:122:SER:N	2.04	0.71
1:A:1080:MET:H	1:B:1215:ASN:HD21	1.37	0.71
1:A:750:ASN:HD22	1:A:1084:GLN:HG2	1.55	0.71
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.26	0.71
1:B:775:VAL:HB	1:B:776:PRO:HD3	1.73	0.70
1:A:82:THR:HG21	1:A:157:HIS:HE1	1.56	0.70
1:B:1132:ASN:HD21	1:B:1139:ARG:NH1	1.90	0.70
1:A:874:GLU:HG2	1:B:66:GLY:HA2	1.73	0.70
1:A:27:ILE:HG22	1:A:28:TYR:N	2.06	0.70
1:A:297:ILE:HB	1:A:379:TYR:CE2	2.26	0.70
1:A:606:VAL:O	1:A:610:VAL:HG23	1.92	0.70
1:A:710:LYS:H	1:A:710:LYS:HD2	1.57	0.70
1:A:467:HIS:CD2	1:A:481:VAL:H	2.10	0.69
1:A:94:ILE:HB	1:A:95:PRO:HD3	1.73	0.69
1:A:1129:MET:HE3	1:A:1149:ARG:HD3	1.74	0.69
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.41	0.69
1:A:526:LEU:O	1:A:531:LYS:HE3	1.91	0.68
1:B:1040:VAL:HG12	1:B:1048:GLN:HE22	1.58	0.68
1:A:1083:SER:O	1:A:1087:MET:HG3	1.93	0.68
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.93	0.68
1:B:174:PHE:HA	1:B:178:HIS:HB2	1.76	0.68
1:A:575:PRO:HG2	1:A:578:LYS:HB3	1.76	0.68
1:A:708:LEU:HD21	1:A:731:LEU:HD22	1.76	0.67
1:A:1108:GLN:HE21	1:A:1110:LYS:HD2	1.59	0.67
1:B:209:ASN:OD1	1:B:211:GLU:HB2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1043:GLY:HA2	1:B:1084:GLN:HE21	1.59	0.67
1:A:857:ARG:HG3	1:A:858:LEU:HD12	1.74	0.67
1:B:5:MET:CE	1:B:184:GLU:HB2	2.24	0.67
1:B:926:TYR:O	1:B:930:LEU:HD13	1.94	0.67
1:A:147:GLN:HE22	1:A:184:GLU:N	1.90	0.67
1:B:224:ILE:HA	1:B:227:GLN:OE1	1.95	0.67
1:A:143:SER:OG	1:A:171:PHE:HB3	1.93	0.67
1:B:398:VAL:HG13	1:B:656:VAL:HG23	1.76	0.67
1:A:27:ILE:HD12	1:A:27:ILE:N	2.09	0.67
1:B:691:GLN:NE2	1:B:727:LYS:H	1.92	0.67
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.41	0.66
1:A:497:ILE:HG13	1:A:498:TYR:HD1	1.60	0.66
1:A:897:ALA:HB3	1:A:910:LEU:HD21	1.77	0.66
1:A:889:HIS:O	1:A:893:LEU:HD13	1.95	0.66
1:A:1019:ARG:NH1	1:B:1180:GLY:HA3	2.06	0.66
1:B:279:SER:O	1:B:283:ILE:HG13	1.95	0.66
1:B:1230:THR:O	1:B:1232:LYS:HG2	1.96	0.66
1:A:51:ILE:HB	1:A:192:ALA:HB2	1.76	0.66
1:A:10:GLY:O	1:A:14:THR:HG23	1.96	0.66
1:A:770:GLN:O	1:A:774:GLN:HG2	1.96	0.66
1:B:1156:LEU:HD12	1:B:1157:ASP:N	2.10	0.66
1:A:27:ILE:HG22	1:A:28:TYR:H	1.59	0.66
1:B:578:LYS:O	1:B:582:LEU:HD13	1.95	0.66
1:B:594:LYS:NZ	1:B:594:LYS:HB3	2.11	0.66
1:B:345:CYS:O	1:B:349:VAL:HG13	1.96	0.66
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.14	0.65
1:A:227:GLN:HE22	1:B:368:LYS:NZ	1.95	0.65
1:B:437:ALA:O	1:B:441:ILE:HG12	1.95	0.65
1:A:128:GLN:NE2	1:B:229:ARG:HE	1.95	0.65
1:A:530:ILE:O	1:A:534:ILE:HG12	1.96	0.65
1:B:817:GLU:HB3	1:B:989:MET:CE	2.24	0.65
1:A:264:VAL:HG11	1:A:284:GLU:HG3	1.78	0.65
1:A:297:ILE:HD13	1:A:297:ILE:H	1.62	0.65
1:A:737:ARG:NH1	1:A:739:GLN:HE22	1.94	0.65
1:B:790:VAL:HG13	1:B:791:LEU:H	1.60	0.65
1:A:840:CYS:SG	1:A:996:ASN:HB3	2.36	0.64
1:B:210:PRO:O	1:B:213:PRO:HD3	1.97	0.64
1:B:1029:VAL:HG23	1:B:1037:VAL:HG21	1.80	0.64
1:A:713:GLU:OE1	1:A:785:PRO:HD2	1.98	0.64
1:A:774:GLN:HE21	1:A:774:GLN:HA	1.63	0.64
1:B:1082:LYS:O	1:B:1086:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LYS:HB2	1:B:262:ASP:OD2	1.98	0.64
1:A:639:PHE:CD1	1:A:643:VAL:HG21	2.32	0.64
1:B:180:ILE:HD13	1:B:180:ILE:C	2.18	0.64
1:A:750:ASN:ND2	1:A:1084:GLN:HG2	2.13	0.63
1:A:594:LYS:HB2	1:A:598:ILE:HD12	1.80	0.63
1:B:823:VAL:HG21	1:B:1049:PHE:CE2	2.31	0.63
1:A:467:HIS:CE1	1:A:480:LEU:HD22	2.32	0.63
1:A:1006:PRO:HG2	1:A:1009:ALA:HB2	1.80	0.63
1:B:5:MET:HE1	1:B:184:GLU:HB2	1.80	0.63
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.81	0.63
1:A:390:PHE:HB2	1:A:403:LEU:HD13	1.81	0.63
1:A:969:ILE:HG23	1:A:970:GLY:N	2.14	0.63
1:B:1181:LYS:HG3	1:B:1182:ALA:H	1.62	0.63
1:B:147:GLN:HE22	1:B:184:GLU:H	1.46	0.63
1:A:271:ARG:HB3	1:A:382:MET:HE3	1.79	0.63
1:A:1015:ALA:HB1	1:B:1185:SER:HB2	1.81	0.62
1:B:91:LEU:HD11	1:B:116:ILE:HD12	1.81	0.62
1:B:593:LYS:CD	1:B:594:LYS:HG3	2.29	0.62
1:A:346:SER:HA	1:A:349:VAL:CG1	2.28	0.62
1:A:1094:GLY:HA3	1:A:1120:PRO:HG3	1.81	0.62
1:B:456:ASP:OD2	1:B:457:SER:N	2.32	0.62
1:B:239:VAL:HG13	1:B:240:PRO:CD	2.23	0.62
1:B:731:LEU:CD2	1:B:790:VAL:HG21	2.29	0.62
1:A:487:VAL:CG2	1:A:504:ILE:HD13	2.29	0.62
1:A:561:MET:HE3	1:A:564:GLN:HB3	1.81	0.62
1:A:1201:PRO:HG3	1:B:455:TYR:HB2	1.79	0.62
1:B:287:ILE:HD11	1:B:379:TYR:OH	1.98	0.62
1:B:835:ALA:HB3	1:B:959:ILE:HG12	1.81	0.62
1:A:467:HIS:HD2	1:A:481:VAL:H	1.47	0.62
1:B:430:THR:HG22	1:B:434:ASN:ND2	2.14	0.62
1:A:937:GLN:HE21	1:A:939:ASP:H	1.47	0.62
1:A:1019:ARG:HH12	1:B:1180:GLY:CA	2.07	0.62
1:A:1028:MET:HE2	1:B:1028:MET:HB3	1.82	0.62
1:B:8:THR:O	1:B:180:ILE:HA	2.00	0.62
1:B:276:MET:HB2	1:B:302:VAL:CG1	2.30	0.62
1:B:1132:ASN:ND2	1:B:1136:VAL:HG13	2.15	0.62
1:A:759:GLU:CD	1:A:759:GLU:H	2.02	0.62
1:A:691:GLN:HE22	1:A:726:ALA:HA	1.64	0.62
1:A:994:TYR:HD2	3:A:2236:TPP:HM41	1.64	0.62
1:A:818:THR:HA	1:A:821:VAL:HG22	1.80	0.61
1:B:398:VAL:HG22	1:B:656:VAL:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:ILE:HG13	1:B:498:TYR:CD1	2.34	0.61
1:A:609:ALA:O	1:A:613:LEU:HD13	2.00	0.61
1:B:263:TYR:HB2	1:B:316:ALA:HB1	1.82	0.61
1:A:274:VAL:HG21	1:A:324:ILE:HD11	1.83	0.61
1:A:1232:LYS:NZ	1:A:1232:LYS:HB3	2.14	0.61
1:A:338:ASP:HB3	1:A:339:PRO:HD2	1.82	0.61
1:A:497:ILE:HG13	1:A:498:TYR:CD1	2.35	0.61
1:A:639:PHE:CE1	1:A:672:PHE:HB2	2.35	0.61
1:A:99:LYS:HE3	1:B:867:SER:O	2.01	0.60
1:A:368:LYS:NZ	1:B:227:GLN:HE22	1.98	0.60
1:A:1010:VAL:HG21	1:A:1136:VAL:HG23	1.82	0.60
1:B:221:ASN:HB2	1:B:223:ASP:OD1	2.02	0.60
1:B:806:MET:SD	1:B:852:PRO:HB2	2.41	0.60
1:A:356:PRO:O	1:A:358:ILE:HG13	2.02	0.60
1:B:325:THR:HG22	1:B:382:MET:SD	2.41	0.60
1:B:593:LYS:HD3	1:B:594:LYS:HG3	1.83	0.60
1:A:1019:ARG:HH12	1:B:1181:LYS:H	1.48	0.60
1:B:434:ASN:O	1:B:438:ILE:HG12	2.01	0.60
1:B:434:ASN:HB3	1:B:468:LEU:HD11	1.83	0.60
1:A:3:LYS:NZ	1:A:254:THR:HA	2.17	0.60
1:B:1043:GLY:HA3	1:B:1087:MET:HB2	1.83	0.60
1:A:931:LYS:HE2	1:A:949:SER:HB2	1.82	0.60
1:A:976:HIS:CE1	1:B:61:MET:HA	2.36	0.60
1:A:331:LYS:O	1:A:333:PRO:HD3	2.02	0.60
1:A:1017:GLY:HA3	1:A:1137:LEU:HD11	1.84	0.60
1:A:279:SER:O	1:A:283:ILE:HG12	2.02	0.60
1:A:1148:LEU:O	1:A:1152:VAL:HG23	2.01	0.60
1:A:1129:MET:HG3	7:A:2242:HOH:O	2.01	0.60
1:A:1219:THR:HG22	1:A:1221:GLU:N	2.17	0.60
1:B:67:ALA:O	1:B:71:VAL:HG23	2.02	0.60
1:B:27:ILE:HD13	1:B:28:TYR:N	2.17	0.59
1:B:917:LYS:NZ	1:B:917:LYS:HB3	2.16	0.59
1:A:1029:VAL:HG11	1:A:1064:LEU:HD13	1.82	0.59
1:B:509:THR:HG22	1:B:540:LYS:HD3	1.84	0.59
1:B:872:ALA:HB3	1:B:965:TRP:CE2	2.37	0.59
1:B:737:ARG:HH11	1:B:739:GLN:HE22	1.51	0.59
1:A:965:TRP:HA	1:A:969:ILE:CG2	2.33	0.59
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.38	0.59
1:B:606:VAL:O	1:B:610:VAL:HG23	2.03	0.59
1:B:620:ASP:OD1	1:B:623:LYS:HE2	2.03	0.59
1:A:239:VAL:CG1	1:A:240:PRO:HD3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1148:LEU:O	1:B:1152:VAL:HG23	2.02	0.59
1:A:345:CYS:O	1:A:349:VAL:HG12	2.03	0.58
1:A:68:ALA:HB2	1:A:93:MET:HG2	1.83	0.58
1:B:1044:TYR:OH	1:B:1118:LYS:HE2	2.03	0.58
1:A:515:PRO:HA	1:A:545:ASP:OD2	2.04	0.58
1:A:1203:MET:HE3	1:B:995:SER:O	2.03	0.58
1:B:351:ARG:HD2	7:B:2094:HOH:O	2.03	0.58
1:A:286:VAL:HG22	1:A:372:PRO:HB3	1.85	0.58
1:B:1064:LEU:HD21	1:B:1066:ILE:HG13	1.84	0.58
1:B:583:LEU:O	1:B:587:ILE:HG13	2.04	0.58
1:B:1043:GLY:HA2	1:B:1084:GLN:NE2	2.18	0.58
1:A:523:ASP:HA	1:A:531:LYS:HE2	1.86	0.58
1:B:1048:GLN:O	1:B:1052:VAL:HG23	2.04	0.58
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.04	0.57
1:A:124:PHE:CE2	1:B:222:PRO:HD3	2.39	0.57
1:A:883:MET:O	1:A:887:ARG:HG3	2.05	0.57
1:A:1024:ASP:O	1:A:1028:MET:HG3	2.04	0.57
1:B:49:LYS:HD2	1:B:53:GLY:O	2.04	0.57
1:B:82:THR:HG22	1:B:83:THR:N	2.19	0.57
1:A:1200:THR:HG22	1:A:1202:MET:N	2.04	0.57
1:B:746:MET:HB3	1:B:813:SER:OG	2.04	0.57
1:B:892:ASP:OD1	1:B:896:LYS:HE3	2.04	0.57
1:A:511:VAL:HA	1:A:542:TYR:O	2.04	0.57
1:B:1232:LYS:NZ	1:B:1232:LYS:HB3	2.20	0.57
1:A:35:THR:O	1:A:39:GLU:HG2	2.04	0.57
1:A:422:PHE:O	1:A:465:ILE:HA	2.03	0.57
1:A:1133:ARG:HG3	1:A:1134:PHE:CD1	2.39	0.57
1:B:283:ILE:O	1:B:287:ILE:HD13	2.04	0.57
1:B:690:ILE:HG12	2:B:2233:SF4:S2	2.45	0.57
1:B:1151:GLN:O	1:B:1155:GLU:HG3	2.04	0.57
1:A:690:ILE:CD1	1:A:692:CYS:HB3	2.26	0.57
1:A:845:GLY:HA2	1:A:852:PRO:HG3	1.86	0.57
1:A:426:GLY:O	1:A:427:ALA:HB3	2.05	0.57
1:B:94:ILE:HB	1:B:95:PRO:HD3	1.86	0.57
1:A:687:GLU:C	1:A:688:ASN:HD22	2.07	0.57
1:A:838:THR:HB	1:A:869:PHE:HB2	1.86	0.57
1:B:857:ARG:HG3	1:B:858:LEU:HD13	1.87	0.57
1:B:130:ILE:HG13	1:B:131:TYR:N	2.20	0.57
1:B:569:LYS:C	1:B:570:LEU:HD12	2.25	0.57
1:B:765:GLN:HE21	1:B:765:GLN:HA	1.69	0.57
1:B:110:HIS:HE1	1:B:157:HIS:NE2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:NE	1:B:123:ILE:HA	2.20	0.56
1:B:275:SER:O	1:B:302:VAL:HG12	2.05	0.56
1:B:351:ARG:HD3	1:B:353:GLU:HB2	1.87	0.56
1:B:1047:GLN:H	1:B:1047:GLN:HE21	1.51	0.56
1:A:49:LYS:HD2	1:A:53:GLY:O	2.06	0.56
1:A:273:ILE:HG23	1:A:327:LEU:HD13	1.87	0.56
1:A:520:GLU:HG3	1:A:521:ASP:N	2.20	0.56
1:B:86:ALA:HA	1:B:111:VAL:HG23	1.86	0.56
1:B:917:LYS:HZ3	1:B:917:LYS:HB3	1.69	0.56
1:B:394:ILE:HD13	1:B:394:ILE:H	1.70	0.56
1:B:581:ASP:O	1:B:585:LYS:HG2	2.06	0.56
1:B:1007:THR:HG21	1:B:1151:GLN:NE2	2.20	0.56
1:A:263:TYR:HB2	1:A:316:ALA:HB1	1.88	0.56
1:A:1181:LYS:HB2	1:A:1181:LYS:NZ	2.20	0.56
1:B:111:VAL:HG13	1:B:170:PHE:HB3	1.88	0.56
1:B:180:ILE:HD12	1:B:438:ILE:HG21	1.88	0.56
1:B:526:LEU:O	1:B:531:LYS:HE3	2.05	0.56
1:B:837:ALA:HB2	1:B:872:ALA:CB	2.34	0.56
1:A:454:SER:HB2	1:A:465:ILE:HG23	1.88	0.56
1:A:523:ASP:HA	1:A:531:LYS:CE	2.35	0.56
1:B:467:HIS:HD2	1:B:481:VAL:H	1.54	0.56
1:B:906:VAL:O	1:B:910:LEU:HD13	2.06	0.56
1:A:274:VAL:CG2	1:A:324:ILE:HD11	2.36	0.56
1:A:374:MET:O	1:A:378:VAL:HG23	2.05	0.56
1:B:912:GLY:HA3	1:B:926:TYR:CD2	2.41	0.56
1:A:700:PRO:HG2	1:A:814:GLY:HA2	1.87	0.56
1:B:364:GLY:HA2	1:B:368:LYS:HB3	1.88	0.56
1:B:856:ASN:HD21	1:B:860:GLN:HB2	1.70	0.56
1:A:917:LYS:HB3	1:A:917:LYS:HZ3	1.71	0.55
1:B:790:VAL:HG13	1:B:791:LEU:N	2.21	0.55
1:A:965:TRP:HA	1:A:969:ILE:HG22	1.89	0.55
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	1.88	0.55
1:B:522:MET:HG2	1:B:616:PHE:CZ	2.41	0.55
1:B:1064:LEU:CD2	1:B:1066:ILE:HG13	2.35	0.55
1:A:27:ILE:HD13	1:A:58:ILE:HG23	1.87	0.55
1:A:642:VAL:O	1:A:646:ILE:HG13	2.06	0.55
1:A:58:ILE:HD12	1:A:58:ILE:N	2.22	0.55
1:A:81:THR:HG22	1:A:82:THR:N	2.21	0.55
1:A:331:LYS:HD3	1:A:362:ARG:NE	2.21	0.55
1:A:396:ASP:O	1:A:400:GLY:HA2	2.07	0.55
1:A:1029:VAL:HG13	1:A:1037:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:GLN:O	1:B:440:ILE:HG12	2.07	0.55
1:B:841:SER:HA	1:B:844:TRP:CE2	2.42	0.55
1:A:869:PHE:CZ	1:A:969:ILE:HG21	2.41	0.55
1:B:731:LEU:HD23	1:B:790:VAL:HG21	1.89	0.55
1:A:227:GLN:HE22	1:B:368:LYS:HZ1	1.54	0.55
1:B:820:TYR:O	1:B:823:VAL:HG22	2.06	0.55
1:A:906:VAL:O	1:A:910:LEU:HB2	2.06	0.55
1:B:238:LYS:O	1:B:242:ILE:HG12	2.06	0.55
1:A:25:ALA:HB1	1:A:27:ILE:HD11	1.89	0.55
1:A:708:LEU:HD22	1:A:801:PHE:CE1	2.42	0.55
1:A:1100:ARG:HH12	1:A:1114:GLN:NE2	2.03	0.55
1:B:7:THR:HA	1:B:181:GLN:O	2.08	0.55
1:B:208:MET:O	1:B:209:ASN:HB2	2.07	0.55
1:A:239:VAL:HG13	1:A:240:PRO:HD3	1.88	0.54
1:A:969:ILE:HG23	1:A:970:GLY:H	1.72	0.54
1:A:331:LYS:HD3	1:A:362:ARG:CZ	2.37	0.54
1:A:1158:VAL:HG12	1:A:1162:GLU:OE2	2.07	0.54
1:B:124:PHE:HB3	1:B:367:SER:OG	2.07	0.54
1:B:1059:PHE:HA	1:B:1104:ARG:NH2	2.21	0.54
1:A:434:ASN:O	1:A:438:ILE:HG12	2.07	0.54
1:A:512:LEU:HD12	1:A:513:ASN:H	1.73	0.54
1:B:635:THR:HG23	1:B:640:LYS:HG3	1.90	0.54
1:B:741:ASN:C	1:B:741:ASN:HD22	2.11	0.54
1:A:157:HIS:O	1:A:161:ILE:HD13	2.07	0.54
1:B:274:VAL:HG23	1:B:324:ILE:CD1	2.34	0.54
1:A:994:TYR:CE1	1:A:1002:SER:HB3	2.43	0.54
1:B:697:PHE:CD2	1:B:1046:LYS:HD3	2.43	0.54
1:B:803:GLU:O	1:B:805:LEU:HD13	2.08	0.54
1:B:87:SER:HA	1:B:129:ASP:HB3	1.89	0.54
1:A:287:ILE:HD11	1:A:379:TYR:CZ	2.43	0.53
1:A:573:VAL:HG22	7:A:2138:HOH:O	2.08	0.53
1:A:992:GLU:O	1:A:993:VAL:HB	2.08	0.53
1:B:552:ASP:HB2	1:B:608:GLN:HE22	1.73	0.53
1:A:215:VAL:HG11	1:B:851:MET:SD	2.49	0.53
1:A:227:GLN:H	1:A:227:GLN:NE2	2.06	0.53
1:A:487:VAL:O	1:A:510:PHE:HD1	1.92	0.53
1:A:1093:SER:HA	1:A:1121:ASP:OD1	2.08	0.53
1:B:7:THR:O	1:B:8:THR:HG23	2.08	0.53
1:A:365:LEU:HD22	1:B:226:PHE:CE2	2.44	0.53
1:A:734:TYR:C	1:A:735:LYS:HD2	2.28	0.53
1:B:994:TYR:HE1	1:B:1002:SER:HB3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:ALA:O	1:A:1017:GLY:HA2	2.08	0.53
1:B:499:ASP:OD2	1:B:502:GLU:HB2	2.08	0.53
1:A:542:TYR:CD2	1:A:570:LEU:HD21	2.43	0.53
1:B:527:PRO:HB2	1:B:530:ILE:HD13	1.91	0.53
1:B:549:ILE:HD12	1:B:549:ILE:N	2.23	0.53
1:B:593:LYS:HD2	1:B:594:LYS:H	1.72	0.53
1:B:805:LEU:HB2	1:B:825:THR:HB	1.91	0.53
1:A:967:TYR:CG	1:A:1004:ALA:HB2	2.43	0.53
1:B:93:MET:O	1:B:97:MET:HG3	2.09	0.53
1:A:959:ILE:HG13	1:A:986:VAL:HG12	1.91	0.53
1:A:1158:VAL:O	1:A:1162:GLU:HG3	2.09	0.53
1:A:1219:THR:CG2	1:A:1220:SER:N	2.72	0.53
1:B:81:THR:HG22	1:B:82:THR:N	2.23	0.53
1:B:465:ILE:HD13	7:B:2126:HOH:O	2.09	0.53
1:A:737:ARG:HE	1:A:739:GLN:NE2	2.07	0.53
1:B:526:LEU:HD11	1:B:530:ILE:HG21	1.90	0.53
1:B:1064:LEU:C	1:B:1064:LEU:HD23	2.29	0.53
1:A:650:GLN:HB3	1:A:653:LYS:HZ1	1.72	0.53
1:A:695:CYS:HB2	1:A:704:ILE:HD13	1.91	0.53
1:A:837:ALA:HB2	1:A:872:ALA:HB2	1.90	0.53
1:A:1044:TYR:HD1	1:A:1088:ASN:HD22	1.57	0.53
1:B:583:LEU:O	1:B:583:LEU:HD23	2.09	0.53
1:B:912:GLY:HA3	1:B:926:TYR:CE2	2.43	0.53
1:A:194:LEU:HD21	1:A:253:LEU:CD1	2.35	0.52
1:A:425:LEU:HD11	1:A:461:GLY:HA2	1.90	0.52
1:B:1027:ARG:HG2	1:B:1030:MET:HE3	1.90	0.52
1:A:512:LEU:O	1:A:544:ILE:HG22	2.08	0.52
1:A:571:ALA:HB3	7:A:2138:HOH:O	2.09	0.52
1:A:792:PRO:HB2	1:A:795:SER:HB3	1.90	0.52
1:A:808:PHE:N	1:A:808:PHE:CD2	2.77	0.52
1:A:1008:GLY:HA2	1:A:1148:LEU:HD13	1.91	0.52
1:B:1123:SER:O	1:B:1126:GLU:HG2	2.09	0.52
1:A:805:LEU:HD23	1:A:862:PRO:HD3	1.91	0.52
1:B:41:ASP:HA	1:B:58:ILE:HD12	1.91	0.52
1:A:690:ILE:HD12	1:A:690:ILE:O	2.09	0.52
1:B:554:GLY:HA3	1:B:601:MET:HE2	1.92	0.52
1:B:1099:PHE:HB3	1:B:1115:LEU:HD23	1.92	0.52
1:B:286:VAL:HG21	1:B:375:VAL:HB	1.91	0.52
1:B:684:TRP:CH2	1:B:737:ARG:HA	2.45	0.52
1:A:173:GLY:O	1:A:174:PHE:HB2	2.09	0.52
1:B:127:HIS:HB3	1:B:130:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:SER:O	1:B:278:SER:HA	2.10	0.52
1:B:324:ILE:HD12	1:B:325:THR:N	2.25	0.52
1:B:390:PHE:HB2	1:B:403:LEU:HD13	1.91	0.52
1:B:698:VAL:HG13	1:B:1084:GLN:OE1	2.09	0.52
1:A:714:LEU:HD12	1:A:714:LEU:N	2.25	0.52
1:A:774:GLN:HA	1:A:774:GLN:NE2	2.24	0.52
1:B:163:SER:O	1:B:164:ASN:HB2	2.10	0.52
1:B:893:LEU:HB3	1:B:945:ILE:CD1	2.37	0.52
1:B:870:GLU:OE2	1:B:870:GLU:N	2.41	0.52
1:B:554:GLY:C	1:B:556:GLY:H	2.13	0.52
1:B:1029:VAL:HG21	1:B:1064:LEU:HD13	1.92	0.52
1:B:1064:LEU:HD23	1:B:1065:VAL:N	2.25	0.52
1:A:9:ASP:HA	1:A:179:GLU:O	2.10	0.52
1:A:396:ASP:HA	1:A:656:VAL:CG1	2.40	0.52
1:B:883:MET:CE	1:B:955:LYS:HG3	2.40	0.52
1:A:526:LEU:HD11	1:A:530:ILE:HG21	1.92	0.51
1:A:720:ASN:N	1:A:720:ASN:HD22	2.08	0.51
1:B:180:ILE:HD13	1:B:181:GLN:N	2.25	0.51
1:A:27:ILE:CG2	1:A:28:TYR:H	2.23	0.51
1:A:717:ALA:HB2	1:A:780:TYR:CZ	2.45	0.51
1:B:584:LYS:HE2	1:B:603:THR:HG23	1.93	0.51
1:A:691:GLN:HE22	1:A:727:LYS:N	2.09	0.51
1:A:788:SER:HB2	1:A:802:GLN:HE22	1.75	0.51
1:A:968:ASP:OD2	1:A:1003:LYS:NZ	2.44	0.51
1:A:124:PHE:HB3	1:A:367:SER:OG	2.10	0.51
1:A:236:TYR:O	1:A:239:VAL:HG12	2.11	0.51
1:B:887:ARG:NH2	1:B:952:TYR:O	2.42	0.51
1:A:87:SER:HB2	1:A:114:ARG:CG	2.41	0.51
1:A:729:LYS:HD2	1:A:730:GLU:OE2	2.10	0.51
1:B:131:TYR:CD1	1:B:330:THR:HG21	2.45	0.51
1:B:264:VAL:HG11	1:B:284:GLU:HG3	1.92	0.51
1:A:394:ILE:CG2	1:B:227:GLN:HE21	2.24	0.51
1:A:697:PHE:CD2	1:A:1046:LYS:HD3	2.45	0.51
1:A:1019:ARG:CZ	1:B:1181:LYS:H	2.23	0.51
1:A:1077:ARG:HH11	1:A:1077:ARG:CB	2.18	0.51
1:B:422:PHE:O	1:B:465:ILE:HA	2.11	0.51
1:B:1137:LEU:HD12	1:B:1145:ALA:HA	1.92	0.51
1:A:3:LYS:O	1:A:4:LYS:HB2	2.10	0.51
1:A:146:VAL:HG12	1:A:183:ILE:HD13	1.93	0.51
1:A:273:ILE:CD1	1:A:325:THR:HG23	2.39	0.51
1:A:436:GLN:O	1:A:440:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:LYS:HB3	1:A:917:LYS:NZ	2.26	0.51
1:B:82:THR:HG23	1:B:108:VAL:O	2.11	0.51
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.41	0.51
1:B:750:ASN:ND2	1:B:1084:GLN:HG2	2.26	0.51
1:A:45:ALA:CB	1:B:1185:SER:HB3	2.40	0.51
1:A:75:LEU:HB2	1:A:105:LEU:HD13	1.93	0.51
1:A:398:VAL:HG23	1:A:399:THR:N	2.26	0.51
1:A:709:ALA:HB3	1:A:714:LEU:HD11	1.93	0.51
1:A:1200:THR:HG23	1:A:1201:PRO:HD2	1.92	0.51
1:B:327:LEU:HB3	1:B:363:TYR:CE1	2.46	0.51
1:A:26:ALA:C	1:A:27:ILE:HD12	2.32	0.51
1:A:48:ARG:O	1:A:55:THR:HG22	2.11	0.51
1:A:413:THR:HG21	1:A:419:GLN:NE2	2.25	0.51
1:A:555:LEU:HD11	1:A:605:ALA:HB2	1.93	0.51
1:A:597:LYS:O	1:A:601:MET:HG3	2.10	0.51
1:A:726:ALA:HB1	1:A:731:LEU:CB	2.37	0.51
1:A:1040:VAL:HG12	1:A:1052:VAL:HG21	1.92	0.51
1:B:142:ALA:HB2	1:B:170:PHE:CZ	2.46	0.51
1:B:530:ILE:HD12	1:B:530:ILE:N	2.26	0.51
1:A:14:THR:CG2	1:A:149:ALA:HB1	2.41	0.50
1:A:242:ILE:O	1:A:245:GLU:HB3	2.11	0.50
1:A:839:GLY:O	1:A:843:ILE:HG12	2.12	0.50
1:A:1144:ASP:HA	1:A:1147:ARG:HH12	1.75	0.50
1:B:121:LEU:HD12	7:B:2226:HOH:O	2.12	0.50
1:B:486:TYR:OH	1:B:511:VAL:HG11	2.10	0.50
1:B:937:GLN:O	1:B:938:LYS:HD2	2.10	0.50
1:A:198:LYS:HD2	1:A:198:LYS:N	2.08	0.50
1:B:115:ALA:HA	1:B:126:ASP:OD2	2.11	0.50
1:B:914:LEU:CD1	1:B:917:LYS:HZ1	2.16	0.50
1:B:941:LEU:O	1:B:945:ILE:HG12	2.12	0.50
1:A:630:LYS:HD2	1:A:630:LYS:C	2.31	0.50
1:A:1186:VAL:HG12	1:B:1015:ALA:O	2.11	0.50
1:B:1077:ARG:HH11	1:B:1077:ARG:CB	2.08	0.50
1:A:331:LYS:HE3	1:B:230:GLU:OE2	2.11	0.50
1:A:775:VAL:N	1:A:776:PRO:HD2	2.26	0.50
1:B:558:ARG:HA	7:B:2148:HOH:O	2.10	0.50
1:A:27:ILE:CG2	1:A:28:TYR:N	2.73	0.50
1:B:24:VAL:HG12	1:B:25:ALA:N	2.26	0.50
1:B:138:PHE:CE2	1:B:166:PRO:HB2	2.45	0.50
1:A:82:THR:CG2	1:A:157:HIS:HE1	2.22	0.50
1:A:857:ARG:HG3	1:A:858:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:TRP:CH2	1:A:686:PRO:HB3	2.46	0.50
1:A:882:SER:OG	1:B:79:ALA:HB2	2.12	0.50
1:A:1025:LEU:O	1:A:1029:VAL:HG12	2.11	0.50
1:B:642:VAL:O	1:B:645:PRO:HD2	2.12	0.50
1:B:713:GLU:OE1	1:B:785:PRO:HD2	2.11	0.50
1:A:62:GLN:NE2	1:B:973:GLY:HA2	2.26	0.50
1:A:524:LYS:HB2	1:A:524:LYS:NZ	2.26	0.50
1:A:661:ALA:HA	1:B:231:ALA:CB	2.42	0.50
1:A:803:GLU:OE1	1:A:856:ASN:HB2	2.10	0.50
1:B:651:GLY:O	1:B:654:LEU:HB2	2.12	0.50
1:B:812:CYS:HB3	7:B:2210:HOH:O	2.11	0.50
1:A:841:SER:HA	1:A:844:TRP:CZ2	2.47	0.49
1:A:1101:TYR:HA	1:A:1112:PRO:O	2.11	0.49
1:A:131:TYR:O	1:A:134:ARG:HG2	2.12	0.49
1:B:1064:LEU:HD21	1:B:1066:ILE:CG1	2.42	0.49
1:B:135:GLN:CD	1:B:135:GLN:H	2.15	0.49
1:B:173:GLY:O	1:B:174:PHE:HB2	2.13	0.49
1:A:11:ASN:HD21	1:A:177:SER:HB2	1.75	0.49
1:A:216:ARG:O	1:B:865:GLY:HA2	2.12	0.49
7:A:2252:HOH:O	1:B:1132:ASN:HB3	2.13	0.49
1:B:491:ASN:HD22	1:B:492:PRO:HD2	1.77	0.49
1:B:646:ILE:HG21	1:B:849:PRO:HD3	1.93	0.49
1:A:394:ILE:HD13	1:A:394:ILE:H	1.78	0.49
1:B:538:LYS:HE3	7:B:2158:HOH:O	2.12	0.49
1:B:542:TYR:CD2	1:B:570:LEU:HD21	2.47	0.49
1:B:700:PRO:HG2	1:B:814:GLY:HA2	1.94	0.49
1:A:325:THR:HB	1:A:359:LEU:HB2	1.93	0.49
1:A:1003:LYS:HE2	1:A:1023:LYS:HD2	1.93	0.49
1:A:1019:ARG:HH12	1:B:1181:LYS:N	2.08	0.49
1:A:220:GLN:HG2	1:A:224:ILE:HD11	1.95	0.49
1:A:630:LYS:HD2	1:A:630:LYS:O	2.12	0.49
1:A:124:PHE:HB3	1:A:367:SER:CB	2.43	0.49
1:A:351:ARG:O	1:A:353:GLU:HG3	2.12	0.49
1:B:513:ASN:ND2	1:B:546:ALA:HB3	2.27	0.49
1:A:271:ARG:HA	1:A:323:VAL:O	2.13	0.49
1:A:602:ASN:O	1:A:606:VAL:HG23	2.13	0.49
1:A:845:GLY:HA2	1:A:852:PRO:CG	2.43	0.49
1:B:63:SER:HB3	1:B:969:ILE:HG13	1.94	0.49
1:A:494:TYR:HB3	1:A:500:ILE:HD11	1.95	0.49
1:A:639:PHE:CA	1:A:643:VAL:HG22	2.41	0.49
1:A:1048:GLN:O	1:A:1052:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:MET:HE3	1:B:564:GLN:HB3	1.94	0.49
1:B:676:GLY:HA2	7:B:2193:HOH:O	2.12	0.49
1:B:986:VAL:O	1:B:986:VAL:HG23	2.13	0.49
1:A:1005:THR:HG23	7:A:2214:HOH:O	2.13	0.48
1:B:331:LYS:HB2	1:B:362:ARG:HD3	1.93	0.48
1:B:844:TRP:O	1:B:852:PRO:HG3	2.13	0.48
1:B:924:LYS:HG2	1:B:928:ASP:OD2	2.13	0.48
1:B:986:VAL:HG22	1:B:1063:SER:O	2.12	0.48
1:A:82:THR:HG21	1:A:157:HIS:CE1	2.43	0.48
1:A:823:VAL:HG11	1:A:1049:PHE:HE2	1.78	0.48
1:B:619:PRO:HG2	1:B:622:TRP:CD1	2.47	0.48
1:B:910:LEU:O	1:B:914:LEU:HD23	2.13	0.48
1:B:1219:THR:HG22	1:B:1220:SER:N	2.27	0.48
1:B:220:GLN:HE21	1:B:225:TYR:HA	1.77	0.48
1:B:573:VAL:O	1:B:574:LEU:HD23	2.13	0.48
1:A:1012:LYS:O	1:A:1013:PHE:HB2	2.12	0.48
1:B:10:GLY:O	1:B:14:THR:HG23	2.13	0.48
1:B:730:GLU:N	1:B:730:GLU:OE1	2.46	0.48
1:A:29:PRO:HB3	1:A:1000:GLN:HG2	1.94	0.48
1:A:368:LYS:HZ1	1:B:227:GLN:HE22	1.61	0.48
1:A:394:ILE:HB	1:B:227:GLN:HG3	1.93	0.48
1:A:688:ASN:HD22	1:A:688:ASN:N	2.10	0.48
1:A:841:SER:HA	1:A:844:TRP:CE2	2.48	0.48
1:B:111:VAL:HG13	1:B:170:PHE:CB	2.43	0.48
1:B:591:TYR:C	1:B:593:LYS:H	2.15	0.48
1:A:686:PRO:HG3	1:A:722:THR:HG21	1.96	0.48
1:A:637:GLU:O	1:A:641:ASN:HB2	2.14	0.48
1:A:1059:PHE:CD1	1:A:1060:PRO:HD2	2.48	0.48
1:B:396:ASP:H	1:B:402:SER:HB3	1.78	0.48
1:B:530:ILE:O	1:B:534:ILE:HG13	2.13	0.48
1:A:70:ALA:HA	1:B:874:GLU:O	2.14	0.48
1:A:1144:ASP:HA	1:A:1147:ARG:NH1	2.29	0.48
1:B:351:ARG:HD3	1:B:353:GLU:OE2	2.14	0.48
1:A:181:GLN:HA	1:A:449:ALA:O	2.13	0.48
1:A:463:ILE:HD11	1:A:649:GLN:NE2	2.29	0.48
1:A:523:ASP:HA	1:A:531:LYS:NZ	2.28	0.48
1:A:573:VAL:HG23	1:A:574:LEU:HG	1.96	0.48
1:A:650:GLN:CD	1:A:653:LYS:HZ1	2.17	0.48
1:A:691:GLN:HE22	1:A:727:LYS:H	1.61	0.48
1:A:720:ASN:HD22	1:A:720:ASN:H	1.60	0.48
1:B:766:PRO:HB2	1:B:769:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:NE	1:A:123:ILE:HA	2.29	0.48
1:A:569:LYS:HD2	1:A:610:VAL:HG13	1.96	0.48
1:B:584:LYS:HA	1:B:587:ILE:HD12	1.96	0.48
1:A:1222:GLN:NE2	1:B:752:ALA:HB3	2.29	0.47
1:A:643:VAL:O	1:A:647:LEU:HG	2.14	0.47
1:B:14:THR:CG2	1:B:149:ALA:HB1	2.44	0.47
1:B:309:VAL:HG12	1:B:312:ALA:H	1.78	0.47
1:B:324:ILE:HG23	1:B:358:ILE:HD13	1.96	0.47
1:A:121:LEU:HD23	1:A:122:SER:N	2.28	0.47
1:A:927:GLY:O	1:A:931:LYS:HG3	2.15	0.47
1:A:1165:HIS:CD2	1:B:1165:HIS:NE2	2.82	0.47
1:B:467:HIS:CE1	1:B:480:LEU:HD22	2.50	0.47
1:B:949:SER:HA	1:B:952:TYR:CE1	2.50	0.47
1:A:720:ASN:H	1:A:720:ASN:ND2	2.12	0.47
1:B:698:VAL:HG11	1:B:1084:GLN:HG3	1.95	0.47
1:B:1019:ARG:NE	1:B:1148:LEU:HD11	2.29	0.47
1:A:113:ALA:HB1	1:A:126:ASP:O	2.14	0.47
1:A:645:PRO:O	1:A:650:GLN:HB2	2.14	0.47
1:B:180:ILE:CD1	1:B:438:ILE:HG21	2.44	0.47
1:B:451:GLY:HA2	1:B:468:LEU:HD23	1.97	0.47
1:B:695:CYS:HB2	1:B:704:ILE:HD13	1.96	0.47
1:B:963:ASP:HB2	1:B:1004:ALA:CB	2.45	0.47
1:B:558:ARG:HG3	1:B:558:ARG:HH11	1.78	0.47
1:B:642:VAL:C	1:B:645:PRO:HD2	2.35	0.47
1:B:1056:ALA:HB1	1:B:1063:SER:HB3	1.95	0.47
1:A:22:SER:O	1:A:56:LEU:HD13	2.15	0.47
1:A:209:ASN:HB3	1:A:212:HIS:CE1	2.49	0.47
1:A:569:LYS:HD3	1:A:613:LEU:HD23	1.96	0.47
1:A:872:ALA:HB3	1:A:965:TRP:CE2	2.50	0.47
1:B:5:MET:HE2	1:B:184:GLU:HB2	1.96	0.47
1:B:278:SER:HB2	1:B:478:THR:HG21	1.96	0.47
1:A:20:ALA:O	1:A:51:ILE:HG23	2.14	0.47
1:A:45:ALA:HB1	1:B:1185:SER:HB3	1.96	0.47
1:A:418:ILE:HD12	1:A:418:ILE:N	2.30	0.47
1:A:648:THR:O	1:A:650:GLN:HG2	2.15	0.47
1:B:397:ASP:OD1	1:B:655:PRO:HB2	2.15	0.47
1:B:591:TYR:C	1:B:593:LYS:N	2.68	0.47
1:B:491:ASN:HD22	1:B:492:PRO:CD	2.28	0.47
1:B:821:VAL:HG23	1:B:822:ARG:N	2.29	0.47
1:B:823:VAL:CG2	1:B:1049:PHE:HE2	2.23	0.47
1:A:691:GLN:NE2	1:A:727:LYS:H	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:VAL:O	1:B:324:ILE:HD12	2.14	0.47
1:B:487:VAL:O	1:B:510:PHE:HD1	1.97	0.47
1:B:668:GLY:HA2	7:B:2169:HOH:O	2.13	0.47
1:B:737:ARG:NH1	1:B:739:GLN:HE22	2.12	0.47
1:B:830:GLU:HB2	1:B:860:GLN:NE2	2.30	0.47
1:A:484:ALA:O	1:A:504:ILE:HD12	2.15	0.46
1:A:750:ASN:OD1	1:A:1081:GLY:HA2	2.15	0.46
1:A:839:GLY:HA2	3:A:2236:TPP:S1	2.55	0.46
1:B:720:ASN:N	1:B:720:ASN:HD22	2.13	0.46
1:B:1044:TYR:CD2	1:B:1091:VAL:HG11	2.50	0.46
1:A:286:VAL:CG2	1:A:372:PRO:HB3	2.45	0.46
1:A:967:TYR:CD2	1:A:1004:ALA:HB2	2.50	0.46
1:A:121:LEU:HD23	1:A:121:LEU:C	2.35	0.46
1:A:129:ASP:OD2	1:A:130:ILE:N	2.45	0.46
1:A:570:LEU:N	1:A:570:LEU:HD12	2.30	0.46
1:A:717:ALA:HB2	1:A:780:TYR:CE2	2.51	0.46
1:A:949:SER:HA	1:A:952:TYR:CZ	2.51	0.46
1:A:1044:TYR:HD1	1:A:1088:ASN:ND2	2.12	0.46
1:A:1102:ASP:OD1	1:A:1104:ARG:CG	2.60	0.46
1:A:1132:ASN:OD1	1:A:1136:VAL:HG13	2.14	0.46
1:A:204:ARG:HG2	1:A:204:ARG:HH21	1.81	0.46
1:A:682:PRO:HG2	1:A:740:ILE:HD12	1.96	0.46
1:B:20:ALA:O	1:B:50:ASN:HB2	2.15	0.46
1:B:272:VAL:HG12	1:B:273:ILE:N	2.30	0.46
1:B:981:GLY:C	1:B:1062:PRO:HD3	2.36	0.46
1:A:499:ASP:OD2	1:A:502:GLU:HB2	2.16	0.46
1:B:595:GLY:C	1:B:597:LYS:H	2.17	0.46
1:A:456:ASP:OD2	1:A:457:SER:N	2.49	0.46
1:A:876:GLY:HA3	1:A:959:ILE:CD1	2.44	0.46
1:A:1082:LYS:O	1:A:1086:VAL:HG23	2.16	0.46
1:B:233:ASN:N	1:B:234:PRO:CD	2.79	0.46
1:B:418:ILE:N	1:B:418:ILE:HD12	2.30	0.46
1:A:527:PRO:O	1:A:531:LYS:HG3	2.15	0.46
1:A:921:ILE:N	1:A:921:ILE:HD12	2.30	0.46
1:B:461:GLY:O	1:B:675:ARG:NH2	2.49	0.46
1:A:9:ASP:OD2	1:A:12:THR:HG23	2.15	0.46
1:A:553:VAL:HG23	1:A:555:LEU:HG	1.97	0.46
1:A:1047:GLN:CD	1:A:1047:GLN:H	2.18	0.46
1:B:500:ILE:HG22	1:B:501:LEU:HD12	1.97	0.46
1:A:1105:LEU:O	1:A:1108:GLN:HG2	2.16	0.45
1:B:20:ALA:HB2	1:B:188:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:TRP:CD2	1:B:738:ILE:HB	2.51	0.45
1:B:755:CYS:SG	1:B:761:ALA:HB3	2.57	0.45
1:A:71:VAL:O	1:A:75:LEU:HG	2.16	0.45
1:A:289:HIS:CD2	1:A:412:THR:HG22	2.52	0.45
1:A:639:PHE:HA	1:A:643:VAL:CG2	2.40	0.45
1:B:14:THR:HG21	1:B:171:PHE:CE2	2.51	0.45
1:B:131:TYR:O	1:B:134:ARG:HG2	2.17	0.45
1:B:465:ILE:HG12	1:B:467:HIS:CE1	2.51	0.45
1:A:644:LYS:HB3	1:A:645:PRO:HD3	1.99	0.45
1:A:838:THR:HB	1:A:869:PHE:CB	2.47	0.45
1:A:973:GLY:HA2	1:B:62:GLN:NE2	2.32	0.45
1:B:96:ASN:O	1:B:100:ILE:HG13	2.15	0.45
1:B:123:ILE:O	1:B:174:PHE:HE2	1.99	0.45
1:B:209:ASN:HB3	1:B:212:HIS:CE1	2.52	0.45
1:B:482:ASN:OD1	1:B:483:ARG:HG3	2.15	0.45
1:B:549:ILE:HD12	1:B:549:ILE:H	1.81	0.45
1:B:628:GLU:HG2	7:B:2140:HOH:O	2.15	0.45
1:B:796:LEU:C	1:B:796:LEU:HD23	2.36	0.45
1:A:538:LYS:HD2	1:A:538:LYS:N	2.31	0.45
1:A:1000:GLN:H	1:A:1000:GLN:NE2	2.14	0.45
1:A:1159:ARG:O	1:A:1162:GLU:HB2	2.17	0.45
1:B:611:THR:HG22	1:B:611:THR:O	2.17	0.45
1:B:871:ASP:O	1:B:874:GLU:HG2	2.16	0.45
1:A:520:GLU:HG3	1:A:521:ASP:H	1.80	0.45
1:A:1072:ILE:HD12	1:A:1073:ASN:N	2.32	0.45
7:A:2124:HOH:O	1:B:1199:ASP:HB3	2.15	0.45
1:B:542:TYR:CZ	1:B:615:GLU:HG2	2.51	0.45
1:A:91:LEU:O	1:A:94:ILE:HG12	2.15	0.45
1:B:594:LYS:NZ	1:B:597:LYS:HD3	2.31	0.45
1:B:729:LYS:HB3	1:B:730:GLU:OE1	2.16	0.45
1:B:883:MET:HE2	1:B:955:LYS:HG3	1.98	0.45
1:A:99:LYS:HE2	1:B:117:ALA:HB1	1.98	0.45
1:A:233:ASN:HB2	1:A:234:PRO:HD3	1.99	0.45
1:A:864:TRP:CE3	1:B:215:VAL:HG23	2.52	0.45
1:A:1047:GLN:OE1	1:A:1047:GLN:N	2.46	0.45
1:B:140:MET:O	1:B:304:LEU:HD12	2.16	0.45
1:B:691:GLN:HE22	1:B:726:ALA:HA	1.81	0.45
1:B:714:LEU:N	1:B:714:LEU:HD12	2.31	0.45
1:B:756:PRO:N	1:B:757:PRO:HD2	2.32	0.45
1:B:818:THR:OG1	1:B:819:PRO:HD3	2.16	0.45
1:A:718:PRO:HB2	1:A:720:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.99	0.45
1:B:317:LEU:HD11	1:B:348:PHE:CZ	2.52	0.45
1:A:398:VAL:HG22	1:A:656:VAL:HG11	1.99	0.45
1:B:513:ASN:HB2	1:B:563:MET:CE	2.47	0.45
1:B:325:THR:HA	1:B:359:LEU:O	2.17	0.45
1:B:396:ASP:OD2	1:B:398:VAL:HG22	2.17	0.45
1:B:495:VAL:HG12	1:B:527:PRO:CD	2.47	0.45
1:B:635:THR:OG1	1:B:636:ASN:N	2.49	0.45
1:A:23:GLU:C	1:A:56:LEU:HD12	2.38	0.44
1:A:87:SER:HB2	1:A:114:ARG:HG2	1.99	0.44
1:A:101:SER:HA	1:A:166:PRO:HG3	1.98	0.44
1:A:237:LEU:O	1:A:240:PRO:HD2	2.16	0.44
1:A:344:VAL:O	1:A:347:ALA:HB3	2.16	0.44
1:A:411:ASP:HB2	1:A:483:ARG:HD3	1.98	0.44
1:A:559:ILE:O	1:A:563:MET:HG2	2.17	0.44
1:B:351:ARG:CD	1:B:353:GLU:HB2	2.47	0.44
1:B:1159:ARG:O	1:B:1163:LEU:HG	2.18	0.44
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.52	0.44
1:A:691:GLN:HG2	1:A:736:PHE:CD2	2.52	0.44
1:A:722:THR:O	1:A:737:ARG:NH2	2.50	0.44
1:A:1003:LYS:HE3	1:B:975:ASP:OD1	2.16	0.44
1:A:1027:ARG:O	1:A:1031:THR:HG23	2.17	0.44
1:B:1059:PHE:C	1:B:1061:GLY:H	2.21	0.44
1:A:338:ASP:HB3	1:A:339:PRO:CD	2.45	0.44
1:A:818:THR:OG1	1:A:819:PRO:HD3	2.18	0.44
1:A:996:ASN:HD22	1:A:997:THR:N	2.14	0.44
1:A:1055:GLU:O	1:A:1104:ARG:NH1	2.51	0.44
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.52	0.44
1:B:750:ASN:HD22	1:B:1084:GLN:HG2	1.82	0.44
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.99	0.44
1:A:243:VAL:O	1:A:247:MET:HG3	2.18	0.44
1:A:886:ARG:O	1:A:889:HIS:HB3	2.16	0.44
1:A:918:ASN:HA	1:A:954:LYS:HD2	2.00	0.44
1:B:600:LYS:O	1:B:604:ASP:N	2.48	0.44
1:B:804:PRO:HG2	1:B:807:GLU:OE2	2.17	0.44
1:A:32:PRO:HB2	1:A:178:HIS:CE1	2.52	0.44
1:A:396:ASP:HA	1:A:656:VAL:HG12	2.00	0.44
1:A:559:ILE:HD12	1:A:559:ILE:C	2.38	0.44
1:A:858:LEU:HD12	1:A:858:LEU:N	2.32	0.44
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.52	0.44
1:A:1193:GLU:OE2	1:B:1077:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:TYR:O	1:B:593:LYS:N	2.50	0.44
1:A:190:ASP:O	1:A:194:LEU:HD23	2.17	0.44
1:B:326:VAL:N	1:B:359:LEU:O	2.51	0.44
1:B:667:LEU:HB3	1:B:854:LYS:HA	1.99	0.44
1:A:327:LEU:N	1:A:327:LEU:HD12	2.31	0.44
1:A:411:ASP:HB2	1:A:483:ARG:CD	2.48	0.44
1:B:85:THR:O	1:B:111:VAL:HG23	2.17	0.44
1:B:561:MET:CE	1:B:583:LEU:HD21	2.48	0.44
1:B:949:SER:HA	1:B:952:TYR:CZ	2.53	0.44
1:A:501:LEU:N	1:A:501:LEU:HD12	2.33	0.44
1:B:549:ILE:HG23	1:B:608:GLN:NE2	2.32	0.44
1:B:569:LYS:HE3	1:B:576:PHE:CE2	2.53	0.44
1:A:1145:ALA:HB1	1:A:1149:ARG:NH1	2.29	0.44
1:B:49:LYS:HB3	1:B:53:GLY:HA2	1.99	0.44
1:B:830:GLU:HB2	1:B:860:GLN:HE21	1.83	0.44
1:B:953:THR:HG23	1:B:955:LYS:NZ	2.33	0.44
1:B:1166:MET:O	1:B:1169:THR:HG22	2.18	0.44
1:A:832:MET:HE2	1:A:834:ILE:HD11	1.99	0.43
1:B:124:PHE:HB3	1:B:367:SER:CB	2.48	0.43
1:B:198:LYS:HD2	1:B:198:LYS:N	2.12	0.43
1:B:214:HIS:HB3	7:B:2048:HOH:O	2.17	0.43
1:B:495:VAL:HG11	1:B:526:LEU:HD12	1.99	0.43
1:B:1124:VAL:O	1:B:1128:LEU:HG	2.18	0.43
1:A:222:PRO:HD3	1:B:124:PHE:CD2	2.52	0.43
1:A:963:ASP:HB2	1:A:1004:ALA:CB	2.47	0.43
1:B:738:ILE:HG22	1:B:740:ILE:CD1	2.48	0.43
1:B:1132:ASN:HB2	7:B:2276:HOH:O	2.17	0.43
1:B:1157:ASP:OD2	1:B:1161:LYS:NZ	2.51	0.43
1:B:1199:ASP:CG	1:B:1214:GLN:HE22	2.22	0.43
1:B:23:GLU:O	1:B:56:LEU:HD12	2.18	0.43
1:B:391:THR:HB	1:B:394:ILE:HD11	2.00	0.43
1:B:591:TYR:HA	1:B:593:LYS:HE2	2.00	0.43
1:B:699:CYS:HA	1:B:700:PRO:HD3	1.84	0.43
1:B:1078:LYS:HB2	1:B:1082:LYS:HG3	2.00	0.43
1:A:159:ALA:HA	1:A:242:ILE:CG2	2.48	0.43
1:A:283:ILE:O	1:A:287:ILE:HG12	2.17	0.43
1:A:545:ASP:O	1:A:549:ILE:HG12	2.18	0.43
1:A:699:CYS:HA	1:A:700:PRO:HD3	1.81	0.43
1:A:710:LYS:HD2	1:A:710:LYS:N	2.29	0.43
1:B:363:TYR:O	1:B:365:LEU:HD12	2.18	0.43
1:B:1219:THR:HB	1:B:1222:GLN:CG	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:O	1:A:324:ILE:HA	2.18	0.43
1:A:1181:LYS:HB2	1:A:1181:LYS:HZ3	1.84	0.43
1:B:501:LEU:HD11	1:B:510:PHE:CE2	2.53	0.43
1:B:577:GLU:O	1:B:578:LYS:C	2.56	0.43
1:B:656:VAL:HG23	1:B:657:SER:N	2.33	0.43
1:A:667:LEU:N	1:A:667:LEU:HD12	2.33	0.43
1:A:688:ASN:N	1:A:688:ASN:ND2	2.64	0.43
1:A:969:ILE:CG2	1:A:970:GLY:N	2.82	0.43
1:B:774:GLN:HA	1:B:774:GLN:NE2	2.33	0.43
1:B:967:TYR:CG	1:B:1004:ALA:HB2	2.54	0.43
1:B:1008:GLY:HA2	1:B:1148:LEU:HD13	1.99	0.43
1:A:346:SER:HA	1:A:349:VAL:HG12	2.00	0.43
1:A:575:PRO:O	1:A:576:PHE:C	2.57	0.43
1:A:686:PRO:HG2	1:A:687:GLU:OE2	2.19	0.43
1:A:1231:LYS:HG3	1:A:1232:LYS:N	2.25	0.43
1:B:1012:LYS:O	1:B:1013:PHE:CB	2.66	0.43
1:B:1052:VAL:HG22	1:B:1100:ARG:HD3	2.00	0.43
1:A:24:VAL:O	1:A:81:THR:HA	2.19	0.43
1:A:68:ALA:HB2	1:A:93:MET:CG	2.48	0.43
1:A:126:ASP:OD2	1:A:126:ASP:C	2.57	0.43
1:A:231:ALA:HB1	1:B:661:ALA:HA	2.00	0.43
1:A:673:GLU:O	1:A:674:LYS:C	2.56	0.43
1:A:909:ALA:HA	1:A:926:TYR:CD2	2.43	0.43
1:A:994:TYR:O	1:A:999:GLY:HA2	2.19	0.43
1:A:1022:LYS:HD2	7:A:2215:HOH:O	2.18	0.43
1:B:595:GLY:C	1:B:597:LYS:N	2.71	0.43
1:A:721:PHE:CZ	1:A:781:ALA:HB2	2.54	0.43
1:A:832:MET:CE	1:A:834:ILE:HD11	2.48	0.43
1:A:973:GLY:O	1:A:977:VAL:HG23	2.19	0.43
1:A:1072:ILE:HA	7:A:2226:HOH:O	2.19	0.43
1:B:68:ALA:HB2	1:B:93:MET:HG2	2.00	0.43
1:B:111:VAL:O	1:B:170:PHE:HA	2.19	0.43
1:B:431:VAL:CG1	1:B:435:LYS:HE3	2.49	0.43
1:B:1232:LYS:HB3	1:B:1232:LYS:HZ2	1.83	0.43
1:A:87:SER:OG	1:A:88:GLN:N	2.52	0.43
1:A:214:HIS:HB3	7:A:2045:HOH:O	2.18	0.43
1:A:668:GLY:HA2	7:A:2186:HOH:O	2.19	0.43
1:A:779:GLU:HA	1:A:779:GLU:OE1	2.18	0.43
1:A:949:SER:HA	1:A:952:TYR:CE2	2.54	0.43
1:A:961:GLY:HA3	1:A:965:TRP:CE3	2.54	0.43
1:A:1156:LEU:HD12	1:A:1157:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASN:HD21	1:B:177:SER:HB2	1.80	0.43
1:B:491:ASN:HD22	1:B:491:ASN:C	2.23	0.43
1:A:297:ILE:HD13	1:A:297:ILE:N	2.28	0.42
1:A:679:ILE:HB	1:B:1216:ARG:O	2.19	0.42
1:A:679:ILE:N	1:A:679:ILE:HD12	2.33	0.42
1:A:914:LEU:HD12	1:A:917:LYS:HZ1	1.83	0.42
1:B:740:ILE:N	1:B:740:ILE:HD12	2.34	0.42
1:B:839:GLY:O	1:B:840:CYS:C	2.58	0.42
1:B:1094:GLY:HA3	1:B:1120:PRO:HG3	2.00	0.42
1:A:710:LYS:HG2	1:A:712:GLU:HB2	2.01	0.42
1:A:821:VAL:HG23	1:A:822:ARG:N	2.34	0.42
1:A:1219:THR:HG22	1:A:1220:SER:N	2.34	0.42
1:A:1230:THR:O	1:A:1231:LYS:C	2.58	0.42
1:B:594:LYS:HB3	1:B:594:LYS:HZ3	1.81	0.42
1:A:188:TYR:HA	1:A:191:MET:HE3	2.00	0.42
1:A:264:VAL:HG11	1:A:284:GLU:CG	2.47	0.42
1:A:861:GLY:O	1:B:210:PRO:HA	2.19	0.42
1:A:1010:VAL:HG21	1:A:1136:VAL:CG2	2.47	0.42
1:A:1211:ALA:HA	1:B:427:ALA:O	2.19	0.42
1:B:729:LYS:C	1:B:729:LYS:HD3	2.39	0.42
1:A:130:ILE:C	1:A:130:ILE:HD12	2.40	0.42
1:A:1200:THR:HG23	1:A:1201:PRO:CD	2.50	0.42
1:A:229:ARG:HH21	1:B:128:GLN:NE2	2.17	0.42
1:A:283:ILE:HB	1:A:299:LEU:HD22	2.02	0.42
1:A:871:ASP:HA	1:A:874:GLU:OE2	2.19	0.42
1:A:1129:MET:HE1	1:A:1149:ARG:NH1	2.35	0.42
1:B:129:ASP:OD2	1:B:130:ILE:N	2.48	0.42
1:B:1105:LEU:HD11	1:B:1114:GLN:NE2	2.35	0.42
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.17	0.42
1:A:674:LYS:HD3	1:A:744:ASP:OD2	2.20	0.42
1:B:368:LYS:HD3	7:B:2099:HOH:O	2.17	0.42
1:B:515:PRO:HA	1:B:545:ASP:OD2	2.20	0.42
1:B:656:VAL:C	1:B:658:ALA:H	2.22	0.42
1:A:368:LYS:NZ	1:B:227:GLN:NE2	2.66	0.42
1:A:661:ALA:HA	1:B:231:ALA:HB1	2.02	0.42
1:A:805:LEU:HD23	1:A:861:GLY:HA2	1.99	0.42
1:A:986:VAL:HG22	1:A:1064:LEU:HA	2.02	0.42
1:B:316:ALA:O	1:B:318:PRO:HD3	2.20	0.42
1:B:783:ARG:O	1:B:785:PRO:HD3	2.19	0.42
1:B:1044:TYR:HA	1:B:1088:ASN:ND2	2.35	0.42
1:A:287:ILE:HD12	1:A:297:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:GLN:HE21	1:A:774:GLN:CA	2.28	0.42
1:A:27:ILE:HD13	1:A:58:ILE:CG2	2.50	0.42
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.49	0.42
1:A:893:LEU:O	1:A:896:LYS:HB2	2.19	0.42
1:A:1078:LYS:HB2	1:A:1082:LYS:HG3	2.01	0.42
1:B:283:ILE:O	1:B:287:ILE:CD1	2.68	0.42
1:B:630:LYS:HE2	1:B:632:GLU:OE2	2.20	0.42
1:B:636:ASN:ND2	1:B:672:PHE:CE1	2.88	0.42
1:B:1071:CYS:O	1:B:1074:GLN:HB2	2.20	0.42
1:B:1156:LEU:HD12	1:B:1156:LEU:C	2.39	0.42
1:A:823:VAL:CG1	1:A:1049:PHE:HE2	2.33	0.42
1:A:994:TYR:CD2	3:A:2236:TPP:HM41	2.49	0.42
1:B:283:ILE:CG2	1:B:299:LEU:HD22	2.50	0.42
1:B:426:GLY:O	1:B:427:ALA:HB3	2.20	0.42
1:B:483:ARG:HG2	1:B:483:ARG:HH11	1.85	0.42
1:A:143:SER:HG	1:A:171:PHE:HB3	1.83	0.41
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.50	0.41
1:A:635:THR:HG23	1:A:640:LYS:HE3	2.02	0.41
1:A:685:VAL:HB	1:A:761:ALA:HA	2.02	0.41
1:B:123:ILE:H	1:B:123:ILE:CD1	2.28	0.41
1:B:583:LEU:HD23	1:B:583:LEU:C	2.40	0.41
1:B:869:PHE:CZ	3:B:2236:TPP:H71	2.54	0.41
1:A:667:LEU:HB3	1:A:854:LYS:HA	2.03	0.41
1:A:896:LYS:HB3	1:A:941:LEU:HD13	2.02	0.41
1:A:1108:GLN:NE2	1:A:1110:LYS:HD2	2.32	0.41
1:A:1193:GLU:CD	1:B:1077:ARG:HG3	2.41	0.41
1:A:1219:THR:HB	1:A:1222:GLN:CG	2.43	0.41
1:B:276:MET:HB2	1:B:302:VAL:HG13	2.00	0.41
1:B:467:HIS:CD2	1:B:481:VAL:H	2.34	0.41
1:B:678:ALA:HB2	1:B:745:CYS:O	2.20	0.41
1:B:695:CYS:O	1:B:704:ILE:HD12	2.20	0.41
1:A:303:ARG:HH21	1:A:303:ARG:HG3	1.85	0.41
1:B:594:LYS:HB3	1:B:594:LYS:HZ2	1.83	0.41
1:A:181:GLN:HE21	1:A:181:GLN:HB3	1.54	0.41
1:A:394:ILE:HG21	1:B:227:GLN:HE21	1.84	0.41
1:A:774:GLN:NE2	1:A:774:GLN:CA	2.83	0.41
1:A:874:GLU:HG2	1:B:66:GLY:CA	2.45	0.41
1:B:609:ALA:O	1:B:613:LEU:HD23	2.20	0.41
1:A:332:GLU:OE2	1:B:135:GLN:HB3	2.21	0.41
1:A:389:HIS:HE1	1:B:350:GLU:OE1	2.03	0.41
1:A:837:ALA:HB2	1:A:872:ALA:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:MET:H	1:B:1215:ASN:HD22	1.63	0.41
1:A:1215:ASN:ND2	1:B:1080:MET:N	2.54	0.41
1:B:30:ILE:O	1:B:30:ILE:HG23	2.20	0.41
1:B:720:ASN:H	1:B:720:ASN:ND2	2.18	0.41
1:B:937:GLN:C	1:B:938:LYS:HD2	2.41	0.41
1:B:994:TYR:HE1	1:B:1002:SER:CB	2.32	0.41
1:A:23:GLU:O	1:A:56:LEU:HD12	2.20	0.41
1:A:349:VAL:HG11	1:B:345:CYS:HB3	2.03	0.41
1:A:562:ILE:N	1:A:562:ILE:HD12	2.36	0.41
1:A:632:GLU:HA	1:A:633:PRO:HD3	1.95	0.41
1:A:756:PRO:HB2	1:A:757:PRO:CD	2.51	0.41
1:B:568:PHE:CD2	1:B:583:LEU:HD12	2.56	0.41
1:A:3:LYS:HB2	7:A:2001:HOH:O	2.20	0.41
1:A:19:TYR:CZ	1:A:48:ARG:HB3	2.56	0.41
1:A:116:ILE:HG12	1:A:128:GLN:HB3	2.00	0.41
1:A:124:PHE:CD2	1:B:222:PRO:HD3	2.55	0.41
1:A:483:ARG:HG2	1:A:483:ARG:HH11	1.86	0.41
1:A:718:PRO:HG2	1:A:777:ASN:ND2	2.36	0.41
1:A:788:SER:HB2	1:A:802:GLN:NE2	2.36	0.41
1:B:1111:ASN:HD21	1:B:1169:THR:HG22	1.86	0.41
1:A:317:LEU:HA	1:A:318:PRO:HD3	1.87	0.41
1:A:520:GLU:HG3	1:A:521:ASP:OD1	2.21	0.41
1:A:690:ILE:HD12	1:A:690:ILE:C	2.41	0.41
1:B:240:PRO:HB3	1:B:309:VAL:HG21	2.02	0.41
1:B:331:LYS:O	1:B:333:PRO:HD3	2.19	0.41
1:B:391:THR:CB	1:B:394:ILE:HD11	2.50	0.41
1:B:803:GLU:OE1	1:B:856:ASN:HB2	2.20	0.41
1:A:99:LYS:O	1:A:103:GLU:HG3	2.20	0.41
1:A:116:ILE:HD11	1:A:129:ASP:HB3	2.03	0.41
1:A:146:VAL:O	1:A:149:ALA:HB3	2.20	0.41
1:A:231:ALA:CB	1:B:661:ALA:HA	2.51	0.41
1:A:306:ARG:HA	1:A:307:PRO:C	2.40	0.41
1:A:546:ALA:C	1:A:559:ILE:HG22	2.41	0.41
1:A:569:LYS:HG2	1:A:570:LEU:HD12	2.03	0.41
1:A:720:ASN:N	1:A:720:ASN:ND2	2.69	0.41
1:B:82:THR:CG2	1:B:83:THR:N	2.84	0.41
1:B:705:LEU:O	1:B:707:VAL:HG23	2.20	0.41
1:A:426:GLY:O	1:A:427:ALA:CB	2.69	0.41
1:A:692:CYS:O	1:A:693:ASN:HB2	2.20	0.41
7:A:2187:HOH:O	1:B:208:MET:HG2	2.20	0.41
1:B:146:VAL:HG12	1:B:183:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:LYS:CE	1:B:603:THR:HG23	2.50	0.41
1:A:887:ARG:HD3	7:A:2196:HOH:O	2.20	0.40
1:B:233:ASN:O	1:B:237:LEU:HG	2.20	0.40
1:B:371:SER:HB2	1:B:372:PRO:HD2	2.03	0.40
1:B:597:LYS:HZ3	1:B:598:ILE:HD13	1.86	0.40
1:B:870:GLU:HB3	1:B:969:ILE:HG12	2.02	0.40
1:A:85:THR:OG1	1:A:86:ALA:N	2.55	0.40
1:A:396:ASP:OD2	1:A:398:VAL:HG22	2.21	0.40
1:B:27:ILE:HD13	1:B:28:TYR:C	2.42	0.40
1:B:180:ILE:C	1:B:180:ILE:CD1	2.88	0.40
1:B:186:LEU:O	1:B:191:MET:HE2	2.21	0.40
1:B:637:GLU:OE1	1:B:637:GLU:N	2.55	0.40
1:B:717:ALA:HA	1:B:780:TYR:CZ	2.57	0.40
1:A:725:GLU:HB3	1:A:735:LYS:NZ	2.36	0.40
1:B:805:LEU:HD23	1:B:862:PRO:HD3	2.03	0.40
1:B:1160:PHE:O	1:B:1164:GLU:N	2.50	0.40
1:A:56:LEU:HB3	1:A:58:ILE:HD11	2.02	0.40
1:A:87:SER:HB2	1:A:114:ARG:HB3	2.03	0.40
1:A:455:TYR:HB3	1:B:1199:ASP:O	2.22	0.40
1:B:7:THR:HG21	1:B:438:ILE:HG22	2.03	0.40
1:B:903:SER:OG	1:B:906:VAL:HG23	2.22	0.40
1:A:51:ILE:CB	1:A:192:ALA:HB2	2.50	0.40
1:A:180:ILE:O	1:A:450:GLN:HA	2.21	0.40
1:A:741:ASN:C	1:A:741:ASN:HD22	2.24	0.40
1:A:918:ASN:CA	1:A:954:LYS:HD2	2.51	0.40
1:B:883:MET:HE1	1:B:955:LYS:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1229/1231 (100%)	1105 (90%)	96 (8%)	28 (2%)	6 16
1	B	1229/1231 (100%)	1120 (91%)	89 (7%)	20 (2%)	9 24
All	All	2458/2462 (100%)	2225 (90%)	185 (8%)	48 (2%)	7 19

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1231	LYS
1	B	556	GLY
1	B	577	GLU
1	B	597	LYS
1	A	4	LYS
1	A	87	SER
1	A	339	PRO
1	A	364	GLY
1	A	623	LYS
1	A	726	ALA
1	B	357	LYS
1	B	578	LYS
1	B	1231	LYS
1	A	993	VAL
1	A	995	SER
1	A	996	ASN
1	A	1015	ALA
1	A	1177	PRO
1	A	1178	ALA
1	A	1182	ALA
1	B	996	ASN
1	B	1177	PRO
1	B	1181	LYS
1	A	104	LEU
1	A	577	GLU
1	A	633	PRO
1	A	674	LYS
1	A	952	TYR
1	B	87	SER
1	B	995	SER
1	A	595	GLY
1	A	711	GLU
1	A	760	LYS
1	A	940	GLY
1	B	339	PRO

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Mol	Chain	Res	Type
1	B	589	LYS
1	B	635	THR
1	B	867	SER
1	B	1060	PRO
1	A	969	ILE
1	B	503	GLY
1	A	440	ILE
1	A	495	VAL
1	B	209	ASN
1	B	364	GLY
1	A	497	ILE
1	A	686	PRO
1	B	715	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	978/978 (100%)	946 (97%)	32 (3%)	38	67
1	B	978/978 (100%)	943 (96%)	35 (4%)	35	64
All	All	1956/1956 (100%)	1889 (97%)	67 (3%)	37	66

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	111	VAL
1	A	141	LEU
1	A	154	LEU
1	A	181	GLN
1	A	226	PHE
1	A	227	GLN
1	A	297	ILE
1	A	303	ARG
1	A	325	THR

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Mol	Chain	Res	Type
1	A	394	ILE
1	A	403	LEU
1	A	491	ASN
1	A	576	PHE
1	A	630	LYS
1	A	632	GLU
1	A	637	GLU
1	A	643	VAL
1	A	710	LYS
1	A	720	ASN
1	A	741	ASN
1	A	759	GLU
1	A	789	GLU
1	A	808	PHE
1	A	917	LYS
1	A	953	THR
1	A	996	ASN
1	A	1000	GLN
1	A	1047	GLN
1	A	1048	GLN
1	A	1088	ASN
1	A	1183	ASP
1	B	8	THR
1	B	27	ILE
1	B	84	PHE
1	B	123	ILE
1	B	154	LEU
1	B	180	ILE
1	B	181	GLN
1	B	211	GLU
1	B	226	PHE
1	B	303	ARG
1	B	317	LEU
1	B	324	ILE
1	B	394	ILE
1	B	491	ASN
1	B	576	PHE
1	B	593	LYS
1	B	624	ASP
1	B	632	GLU
1	B	637	GLU
1	B	643	VAL

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Mol	Chain	Res	Type
1	B	654	LEU
1	B	693	ASN
1	B	720	ASN
1	B	741	ASN
1	B	754	ILE
1	B	789	GLU
1	B	892	ASP
1	B	917	LYS
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1088	ASN
1	B	1118	LYS
1	B	1137	LEU
1	B	1172	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	16	HIS
1	A	46	GLN
1	A	110	HIS
1	A	128	GLN
1	A	147	GLN
1	A	164	ASN
1	A	169	HIS
1	A	212	HIS
1	A	220	GLN
1	A	221	ASN
1	A	227	GLN
1	A	233	ASN
1	A	288	ASN
1	A	289	HIS
1	A	389	HIS
1	A	421	GLN
1	A	434	ASN
1	A	467	HIS
1	A	491	ASN
1	A	513	ASN
1	A	588	HIS
1	A	608	GLN

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Mol	Chain	Res	Type
1	A	614	GLN
1	A	649	GLN
1	A	688	ASN
1	A	691	GLN
1	A	693	ASN
1	A	720	ASN
1	A	739	GLN
1	A	741	ASN
1	A	750	ASN
1	A	770	GLN
1	A	774	GLN
1	A	777	ASN
1	A	802	GLN
1	A	860	GLN
1	A	866	ASN
1	A	918	ASN
1	A	937	GLN
1	A	976	HIS
1	A	1000	GLN
1	A	1048	GLN
1	A	1073	ASN
1	A	1084	GLN
1	A	1088	ASN
1	A	1108	GLN
1	A	1151	GLN
1	A	1154	HIS
1	A	1215	ASN
1	B	11	ASN
1	B	16	HIS
1	B	46	GLN
1	B	54	GLN
1	B	110	HIS
1	B	128	GLN
1	B	147	GLN
1	B	164	ASN
1	B	169	HIS
1	B	181	GLN
1	B	212	HIS
1	B	220	GLN
1	B	221	ASN
1	B	227	GLN
1	B	233	ASN

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Mol	Chain	Res	Type
1	B	248	GLN
1	B	389	HIS
1	B	434	ASN
1	B	467	HIS
1	B	491	ASN
1	B	513	ASN
1	B	536	ASN
1	B	608	GLN
1	B	614	GLN
1	B	636	ASN
1	B	650	GLN
1	B	688	ASN
1	B	691	GLN
1	B	693	ASN
1	B	720	ASN
1	B	739	GLN
1	B	741	ASN
1	B	750	ASN
1	B	765	GLN
1	B	774	GLN
1	B	777	ASN
1	B	836	ASN
1	B	860	GLN
1	B	866	ASN
1	B	918	ASN
1	B	937	GLN
1	B	976	HIS
1	B	996	ASN
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1073	ASN
1	B	1084	GLN
1	B	1088	ASN
1	B	1108	GLN
1	B	1114	GLN
1	B	1132	ASN
1	B	1215	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PYR	B	2239	-	5,5,5	0.98	0	3,6,6	2.12	1 (33%)
2	SF4	A	2233	1	0,12,12	-	-	-		
3	TPP	A	2236	4	22,27,27	4.32	9 (40%)	29,40,40	2.03	7 (24%)
6	PYR	A	2239	-	5,5,5	1.10	0	3,6,6	2.03	1 (33%)
2	SF4	A	2235	1	0,12,12	-	-	-		
2	SF4	B	2233	1	0,12,12	-	-	-		
2	SF4	B	2235	1	0,12,12	-	-	-		
2	SF4	A	2234	1	0,12,12	-	-	-		
2	SF4	B	2234	1	0,12,12	-	-	-		
3	TPP	B	2236	4	22,27,27	3.86	8 (36%)	29,40,40	2.03	8 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PYR	B	2239	-	-	0/4/4/4	-
2	SF4	A	2233	1	-	-	0/6/5/5
3	TPP	A	2236	4	-	6/16/17/17	0/2/2/2
6	PYR	A	2239	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	2235	1	-	-	0/6/5/5
2	SF4	B	2233	1	-	-	0/6/5/5
2	SF4	B	2235	1	-	-	0/6/5/5
2	SF4	A	2234	1	-	-	0/6/5/5
2	SF4	B	2234	1	-	-	0/6/5/5
3	TPP	B	2236	4	-	3/16/17/17	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2236	TPP	C4-N3	12.02	1.50	1.39
3	A	2236	TPP	C4-N3	11.67	1.49	1.39
3	A	2236	TPP	C4'-N3'	8.88	1.47	1.35
3	A	2236	TPP	C6-C5	8.13	1.54	1.50
3	B	2236	TPP	C6'-C5'	6.59	1.51	1.37
3	B	2236	TPP	C2'-N3'	6.33	1.45	1.34
3	A	2236	TPP	C2'-N3'	5.00	1.42	1.34
3	A	2236	TPP	C2'-N1'	4.99	1.42	1.34
3	B	2236	TPP	C4'-N3'	4.90	1.42	1.35
3	B	2236	TPP	C6'-N1'	4.79	1.44	1.34
3	A	2236	TPP	C5'-C4'	4.73	1.51	1.42
3	A	2236	TPP	C6'-N1'	4.61	1.44	1.34
3	B	2236	TPP	C2'-N1'	3.98	1.40	1.34
3	A	2236	TPP	C6'-C5'	3.76	1.45	1.37
3	B	2236	TPP	C5'-C4'	3.62	1.49	1.42
3	A	2236	TPP	CM4-C4	2.64	1.55	1.49
3	B	2236	TPP	PA-O7	-2.20	1.50	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2236	TPP	C6-C5-C4	6.33	132.52	127.43
3	A	2236	TPP	C5'-C7'-N3	5.60	122.59	113.28
3	B	2236	TPP	C5'-C7'-N3	5.14	121.83	113.28
3	A	2236	TPP	C6-C5-C4	4.21	130.82	127.43
3	A	2236	TPP	C6'-N1'-C2'	3.51	121.94	115.96
3	A	2236	TPP	CM2-C2'-N3'	3.50	122.62	117.15
6	B	2239	PYR	OXT-C-CA	3.39	123.24	113.97
3	A	2236	TPP	C7'-N3-C2	-3.30	119.39	125.35
6	A	2239	PYR	OXT-C-CA	3.25	122.86	113.97
3	A	2236	TPP	N1'-C2'-N3'	-3.03	120.32	125.54
3	B	2236	TPP	N1'-C2'-N3'	-2.81	120.70	125.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2236	TPP	C7'-N3-C2	-2.55	120.73	125.35
3	B	2236	TPP	C6'-N1'-C2'	2.23	119.77	115.96
3	A	2236	TPP	O3B-PB-O3A	2.23	112.10	104.64
3	B	2236	TPP	C6'-C5'-C4'	-2.18	112.75	115.72
3	B	2236	TPP	CM4-C4-N3	2.14	125.26	122.53
3	B	2236	TPP	CM2-C2'-N3'	2.09	120.42	117.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2236	TPP	C5-C6-C7-O7
3	A	2236	TPP	C7-O7-PA-O3A
3	B	2236	TPP	C5-C6-C7-O7
3	B	2236	TPP	C7-O7-PA-O1A
3	A	2236	TPP	PB-O3A-PA-O7
3	B	2236	TPP	PB-O3A-PA-O7
3	A	2236	TPP	C7-O7-PA-O1A
3	A	2236	TPP	C7-O7-PA-O2A
3	A	2236	TPP	C4-C5-C6-C7

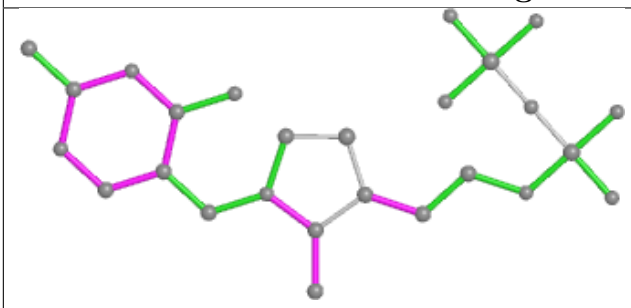
There are no ring outliers.

3 monomers are involved in 5 short contacts:

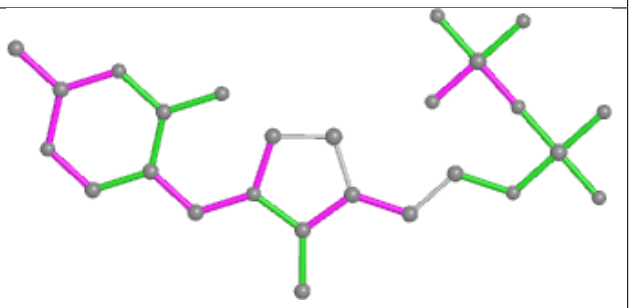
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2236	TPP	3	0
2	B	2233	SF4	1	0
3	B	2236	TPP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

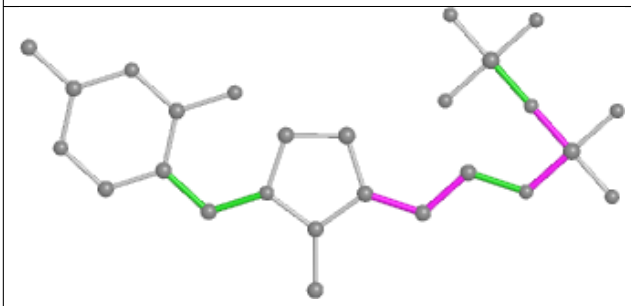
Ligand TPP A 2236



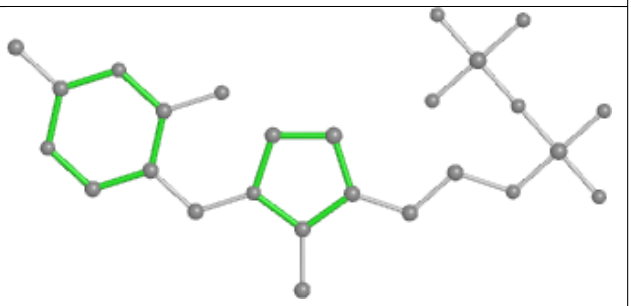
Bond lengths



Bond angles

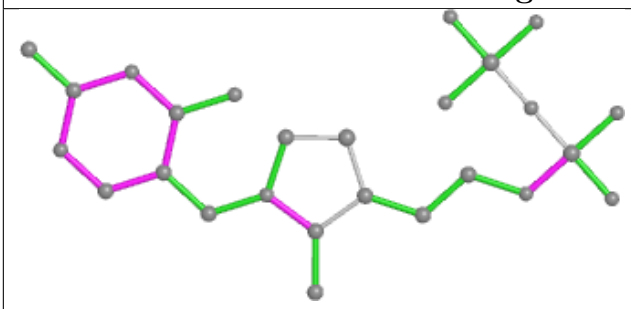


Torsions

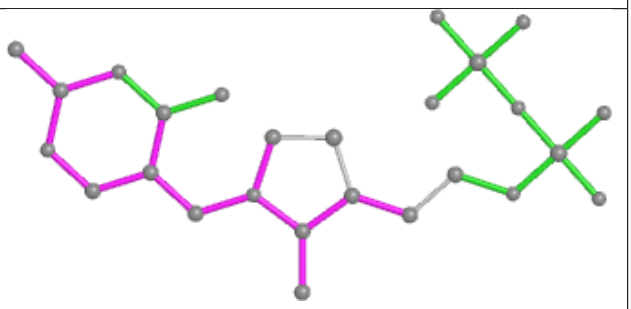


Rings

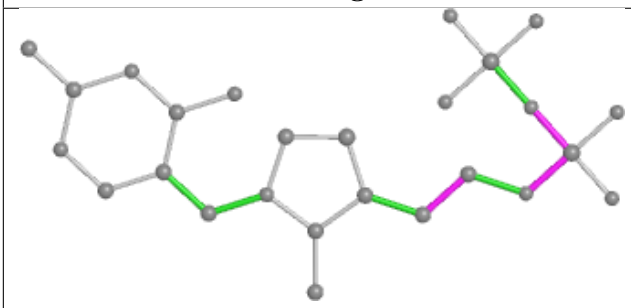
Ligand TPP B 2236



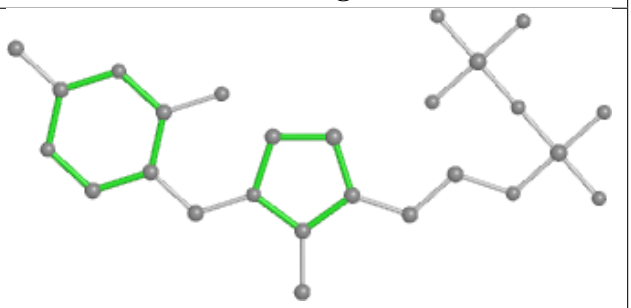
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1231/1231 (100%)	0.08	63 (5%)	28	26	3, 26, 71, 114	0
1	B	1231/1231 (100%)	-0.19	36 (2%)	51	52	2, 18, 55, 117	0
All	All	2462/2462 (100%)	-0.05	99 (4%)	38	37	2, 22, 64, 117	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1180	GLY	7.6
1	B	1182	ALA	7.4
1	A	631	ALA	6.6
1	A	595	GLY	6.3
1	A	626	PRO	5.7
1	A	629	THR	5.6
1	B	1181	LYS	5.5
1	A	408	ALA	5.3
1	B	1232	LYS	5.1
1	B	631	ALA	5.0
1	B	576	PHE	4.9
1	A	1232	LYS	4.7
1	A	593	LYS	4.7
1	A	630	LYS	4.5
1	B	1178	ALA	4.5
1	B	1179	GLY	4.5
1	A	628	GLU	4.5
1	A	575	PRO	4.4
1	A	598	ILE	4.4
1	B	1183	ASP	4.3
1	A	577	GLU	4.2
1	A	574	LEU	4.2
1	A	637	GLU	4.2
1	A	576	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	596	GLU	4.1
1	A	594	LYS	4.1
1	B	1230	THR	3.9
1	A	635	THR	3.9
1	B	593	LYS	3.8
1	A	627	ALA	3.8
1	A	634	MET	3.7
1	B	594	LYS	3.7
1	B	589	LYS	3.7
1	A	581	ASP	3.6
1	A	591	TYR	3.6
1	A	1231	LYS	3.6
1	A	550	ALA	3.6
1	B	629	THR	3.6
1	A	590	ALA	3.6
1	B	591	TYR	3.5
1	A	536	ASN	3.4
1	A	633	PRO	3.3
1	A	768	ASP	3.3
1	B	2	GLY	3.2
1	B	597	LYS	3.2
1	A	1179	GLY	3.2
1	A	731	LEU	3.1
1	A	758	LYS	3.1
1	B	3	LYS	3.1
1	B	1177	PRO	3.1
1	A	538	LYS	3.1
1	B	595	GLY	3.1
1	A	1143	GLU	3.1
1	A	601	MET	3.0
1	B	632	GLU	2.9
1	A	632	GLU	2.9
1	A	625	ALA	2.8
1	A	1140	SER	2.7
1	B	1176	ALA	2.7
1	A	592	GLY	2.7
1	A	1178	ALA	2.7
1	A	520	GLU	2.7
1	A	715	VAL	2.7
1	A	780	TYR	2.6
1	A	727	LYS	2.6
1	A	640	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1231	LYS	2.5
1	B	634	MET	2.5
1	A	582	LEU	2.5
1	A	725	GLU	2.5
1	A	769	THR	2.5
1	B	1228	LYS	2.4
1	A	589	LYS	2.4
1	A	1165	HIS	2.4
1	A	555	LEU	2.4
1	A	552	ASP	2.4
1	A	578	LYS	2.4
1	B	1165	HIS	2.3
1	B	711	GLU	2.3
1	A	783	ARG	2.3
1	B	1221	GLU	2.3
1	A	597	LYS	2.3
1	B	590	ALA	2.3
1	A	624	ASP	2.3
1	A	1145	ALA	2.2
1	A	584	LYS	2.2
1	A	583	LEU	2.2
1	B	1226	LEU	2.2
1	A	607	ASP	2.2
1	A	1119	ALA	2.1
1	B	587	ILE	2.1
1	A	596	GLU	2.1
1	B	1229	ARG	2.1
1	A	641	ASN	2.1
1	B	687	GLU	2.1
1	A	619	PRO	2.0
1	B	790	VAL	2.0
1	A	729	LYS	2.0
1	B	630	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

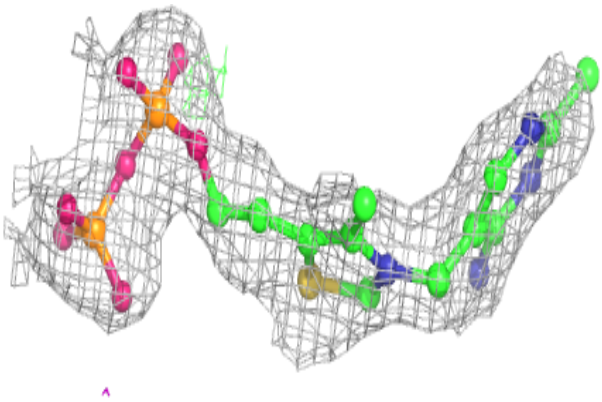
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

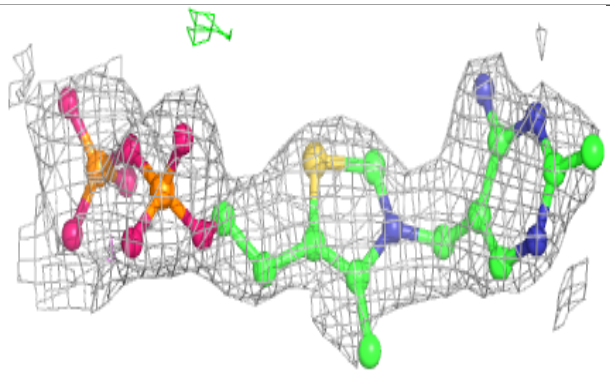
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PYR	A	2239	6/6	0.83	0.29	50,55,57,58	0
5	CA	A	2238	1/1	0.92	0.10	61,61,61,61	0
4	MG	A	2237	1/1	0.94	0.07	16,16,16,16	0
6	PYR	B	2239	6/6	0.94	0.17	17,23,25,26	0
2	SF4	A	2235	8/8	0.96	0.07	20,25,26,28	0
3	TPP	A	2236	26/26	0.96	0.14	23,36,48,52	0
2	SF4	A	2234	8/8	0.97	0.05	28,29,32,33	0
5	CA	B	2238	1/1	0.97	0.10	47,47,47,47	0
3	TPP	B	2236	26/26	0.97	0.13	3,14,23,31	0
2	SF4	A	2233	8/8	0.97	0.10	32,34,36,36	0
2	SF4	B	2234	8/8	0.98	0.05	7,10,12,13	0
2	SF4	B	2235	8/8	0.98	0.05	6,11,12,12	0
2	SF4	B	2233	8/8	0.98	0.04	20,22,24,24	0
4	MG	B	2237	1/1	0.99	0.05	3,3,3,3	0

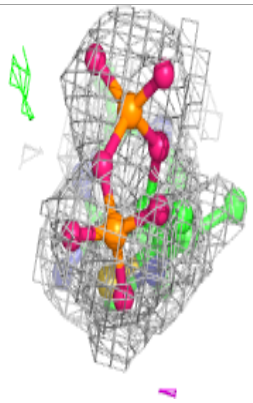
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TPP A 2236:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

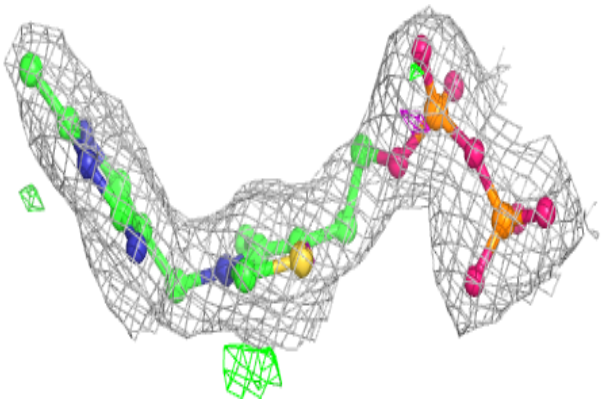


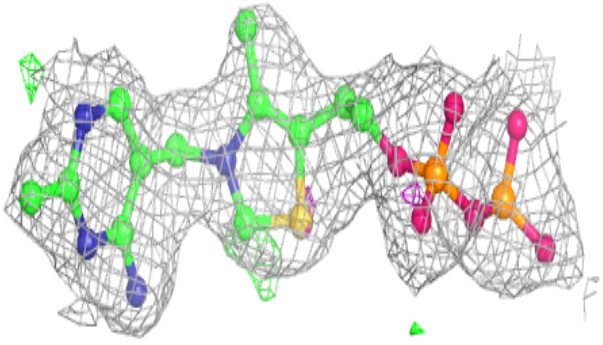


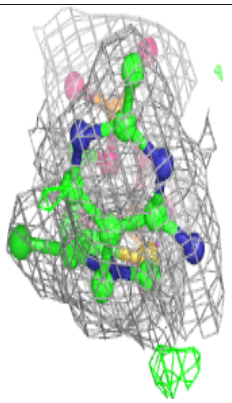


Electron density around TPP B 2236:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.