Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:58 pm BST

PDB ID	:	3VSG
Title	:	Crystal structure of iron free 1,6-APD, 2-Animophenol-1,6-Dioxygenase
Authors	:	Li, D.F.; Hou, Y.J.; Hu, Y.; Wang, D.C.; Liu, W.
Deposited on	:	2012-04-25
Resolution	:	2.40 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 ⓘ symbol.

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

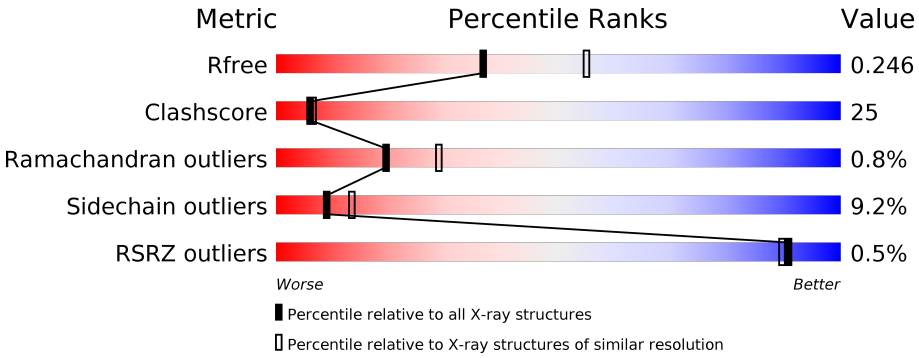
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	271	69% 26% 5%
1	C	271	64% 32% .
2	B	312	% 54% 39% . .
2	D	312	% 49% 39% 8% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10215 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 2-amino-5-chlorophenol 1,6-dioxygenase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2056	1303	358	389	6			
1	C	270	Total	C	N	O	S	0	0	0
			2056	1303	358	389	6			

- Molecule 2 is a protein called 2-amino-5-chlorophenol 1,6-dioxygenase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	304	Total	C	N	O	S	0	0	0
			2410	1541	415	439	15			
2	D	300	Total	C	N	O	S	0	0	0
			2383	1526	410	432	15			

- Molecule 3 is water.

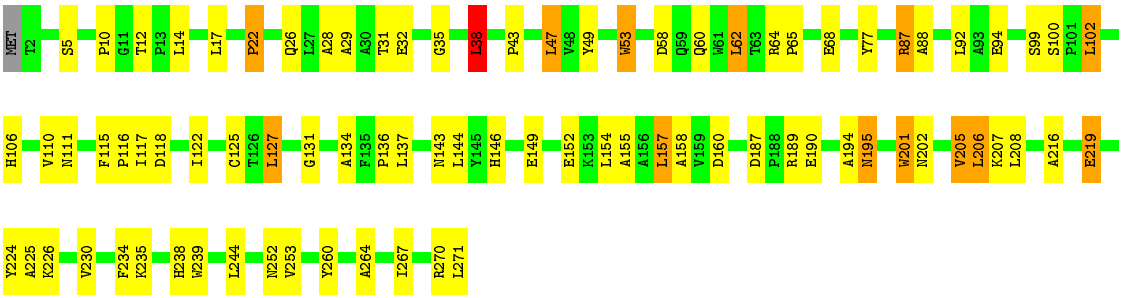
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	398	Total	O	0	0
			398	398		
3	B	293	Total	O	0	0
			293	293		
3	C	330	Total	O	0	0
			330	330		
3	D	289	Total	O	0	0
			289	289		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

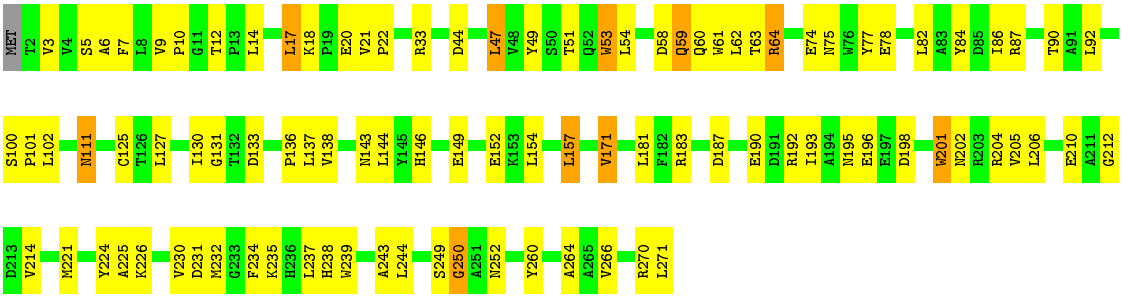
- Molecule 1: 2-amino-5-chlorophenol 1,6-dioxygenase alpha subunit

Chain A:



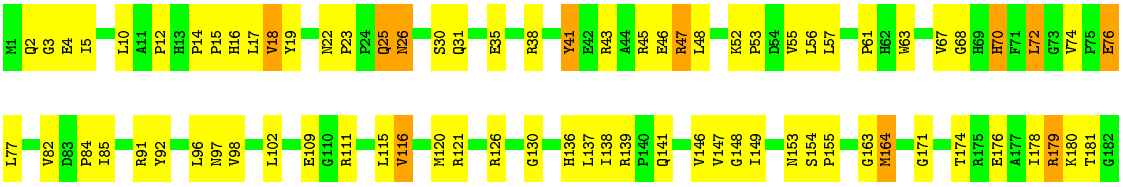
- Molecule 1: 2-amino-5-chlorophenol 1,6-dioxygenase alpha subunit

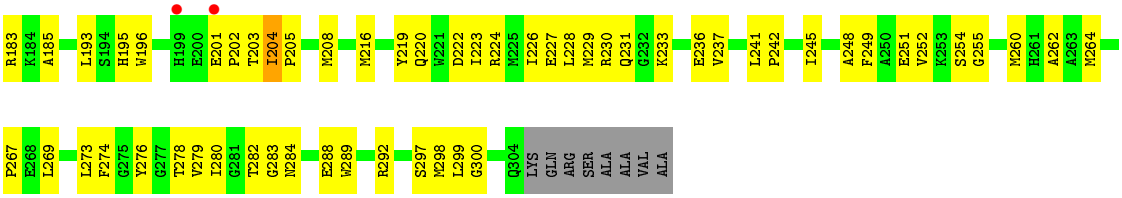
Chain C:



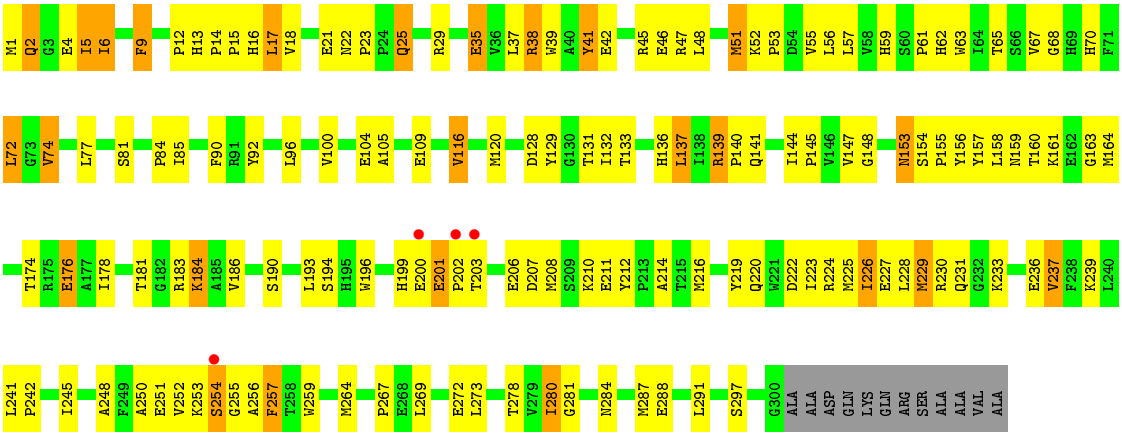
- Molecule 2: 2-amino-5-chlorophenol 1,6-dioxygenase beta subunit

Chain B:





- Molecule 2: 2-amino-5-chlorophenol 1,6-dioxygenase beta subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	269.73Å 48.26Å 108.44Å 90.00° 109.44° 90.00°	Depositor
Resolution (Å)	39.78 – 2.40 39.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.4 (39.78-2.40) 86.4 (39.78-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.247 0.185 , 0.246	Depositor DCC
R_{free} test set	2271 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10215	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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

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	0.40	0/2102	0.70	1/2860 (0.0%)
1	C	0.37	0/2102	0.66	1/2860 (0.0%)
2	B	0.37	0/2478	0.65	1/3364 (0.0%)
2	D	0.39	0/2451	0.67	1/3327 (0.0%)
All	All	0.38	0/9133	0.67	4/12411 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	257	PHE	N-CA-C	-7.26	91.40	111.00
1	C	138	VAL	N-CA-C	-6.00	94.79	111.00
1	A	38	LEU	CA-CB-CG	5.22	127.31	115.30
2	B	10	LEU	N-CA-C	-5.08	97.28	111.00

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	2056	0	2027	69	0
1	C	2056	0	2027	91	0
2	B	2410	0	2359	139	0
2	D	2383	0	2337	161	0
3	A	398	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	293	0	0	18	0
3	C	330	0	0	15	0
3	D	289	0	0	13	0
All	All	10215	0	8750	438	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 25.

All (438) 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)
2:D:256:ALA:HB1	2:D:259:TRP:H	1.28	0.98
1:C:51:THR:HG21	1:C:231:ASP:OD2	1.69	0.93
2:B:14:PRO:HG2	2:B:17:LEU:HG	1.51	0.92
1:C:100:SER:HA	1:C:157:LEU:HD11	1.53	0.90
2:D:139:ARG:HH11	2:D:141:GLN:HB2	1.39	0.87
1:C:47:LEU:HD22	1:C:239:TRP:HZ2	1.44	0.83
2:D:25:GLN:HG3	2:D:92:TYR:CZ	2.13	0.82
1:C:54:LEU:HD22	1:C:144:LEU:HD21	1.62	0.81
2:B:283:GLY:C	2:B:284:ASN:HD22	1.84	0.81
2:B:25:GLN:H	2:B:25:GLN:HE21	1.29	0.80
2:D:222:ASP:O	2:D:226:ILE:HG23	1.82	0.80
1:A:149:GLU:HG2	3:A:394:HOH:O	1.83	0.78
2:B:226:ILE:HD11	2:D:39:TRP:CH2	2.17	0.78
2:B:222:ASP:O	2:B:226:ILE:HG23	1.83	0.78
1:C:192:ARG:HD2	3:C:537:HOH:O	1.83	0.78
2:B:92:TYR:OH	2:B:136:HIS:HD2	1.68	0.77
2:D:17:LEU:HD11	2:D:37:LEU:HB3	1.64	0.77
1:C:47:LEU:HD22	1:C:239:TRP:CZ2	2.20	0.76
2:D:68:GLY:HA3	2:D:116:VAL:HG22	1.68	0.76
2:B:241:LEU:O	2:B:245:ILE:HG12	1.85	0.76
1:C:252:ASN:HD21	1:C:270:ARG:HH11	1.32	0.76
2:D:61:PRO:HB3	2:D:254:SER:HB3	1.67	0.75
1:A:53:TRP:HZ3	1:A:60:GLN:OE1	1.69	0.75
2:B:174:THR:O	2:B:178:ILE:HG12	1.88	0.74
2:D:196:TRP:HE1	2:D:248:ALA:HA	1.51	0.73
2:B:47:ARG:HH11	2:B:47:ARG:HG2	1.53	0.72
2:B:5:ILE:HG12	2:B:299:LEU:HD21	1.73	0.71
1:C:51:THR:HG23	1:C:232:MET:HG3	1.71	0.71
1:C:87:ARG:HD2	3:C:345:HOH:O	1.89	0.71
2:D:56:LEU:HD13	2:D:144:ILE:HG21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:VAL:HG12	3:C:317:HOH:O	1.91	0.70
2:B:67:VAL:O	2:B:70:HIS:HE1	1.73	0.70
2:D:252:VAL:HG23	2:D:257:PHE:HB3	1.73	0.70
2:B:193:LEU:HB2	3:B:511:HOH:O	1.91	0.70
1:A:131:GLY:HA2	1:A:137:LEU:HG	1.73	0.69
1:C:5:SER:HB3	1:C:7:PHE:HE1	1.56	0.69
2:B:245:ILE:CD1	2:B:252:VAL:HG23	2.23	0.69
1:C:244:LEU:HD13	3:C:525:HOH:O	1.93	0.69
1:C:51:THR:HG23	1:C:232:MET:CG	2.23	0.69
2:D:128:ASP:HB3	3:D:476:HOH:O	1.92	0.69
2:D:74:VAL:HG22	2:D:77:LEU:HG	1.75	0.68
1:A:202:ASN:O	1:A:206:LEU:HB2	1.93	0.68
2:B:26:ASN:HD21	2:B:91:ARG:H	1.41	0.68
2:D:9:PHE:HB3	2:D:288:GLU:HA	1.74	0.68
2:D:128:ASP:O	2:D:132:ILE:HG12	1.92	0.68
2:B:226:ILE:O	2:B:230:ARG:HG2	1.95	0.67
2:B:3:GLY:HA3	2:B:179:ARG:HA	1.75	0.67
2:B:280:ILE:HG22	2:B:280:ILE:O	1.95	0.67
1:A:29:ALA:HB3	3:A:497:HOH:O	1.94	0.67
1:A:252:ASN:HB2	3:A:371:HOH:O	1.94	0.67
1:C:51:THR:HG21	1:C:231:ASP:CG	2.14	0.67
2:D:16:HIS:CE1	2:D:280:ILE:HD11	2.29	0.67
2:D:67:VAL:O	2:D:70:HIS:HE1	1.78	0.67
2:B:279:VAL:HG22	2:B:280:ILE:HD13	1.76	0.66
1:C:84:TYR:HB2	1:C:86:ILE:CD1	2.26	0.66
2:B:68:GLY:HA2	2:B:116:VAL:HG13	1.77	0.66
1:C:125:CYS:HA	1:C:130:ILE:HG12	1.76	0.66
2:B:84:PRO:HG2	2:B:85:ILE:HD12	1.78	0.65
1:C:58:ASP:CG	2:D:200:GLU:HG3	2.16	0.65
2:D:133:THR:O	2:D:137:LEU:HD22	1.95	0.65
2:B:25:GLN:NE2	2:B:25:GLN:H	1.93	0.65
2:D:9:PHE:HB2	2:D:287:MET:O	1.97	0.65
2:D:239:LYS:HE3	3:D:466:HOH:O	1.97	0.65
2:D:92:TYR:OH	2:D:136:HIS:HD2	1.80	0.65
2:D:1:MET:O	2:D:2:GLN:HB2	1.97	0.64
1:C:18:LYS:HA	1:C:20:GLU:OE2	1.97	0.64
1:C:252:ASN:HD21	1:C:270:ARG:NH1	1.95	0.64
2:B:139:ARG:CZ	2:B:141:GLN:NE2	2.61	0.64
2:D:14:PRO:HG2	2:D:17:LEU:HG	1.78	0.64
2:D:202:PRO:CB	2:D:210:LYS:HD2	2.27	0.64
2:D:256:ALA:HB1	2:D:259:TRP:N	2.09	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:SER:HB3	1:C:7:PHE:CE1	2.34	0.63
2:D:25:GLN:HG3	2:D:92:TYR:CE1	2.34	0.63
2:D:181:THR:HG22	2:D:183:ARG:NH1	2.14	0.63
1:A:88:ALA:HB3	3:A:383:HOH:O	1.97	0.63
1:A:206:LEU:HD11	1:A:267:ILE:HD11	1.81	0.62
2:B:219:TYR:OH	2:D:35:GLU:HG2	1.99	0.62
2:D:6:ILE:HG21	2:D:51:MET:HG2	1.82	0.62
2:D:62:HIS:HB2	3:D:476:HOH:O	2.00	0.62
1:A:125:CYS:SG	1:A:137:LEU:HD11	2.39	0.62
1:A:47:LEU:HD22	1:A:239:TRP:CZ2	2.34	0.62
2:D:212:TYR:HA	2:D:278:THR:HG21	1.82	0.62
2:B:35:GLU:HG3	2:D:223:ILE:HD12	1.81	0.62
2:B:72:LEU:HD22	2:B:148:GLY:HA3	1.81	0.61
1:C:143:ASN:HB3	1:C:146:HIS:CD2	2.36	0.61
1:C:87:ARG:NE	1:C:133:ASP:HB3	2.16	0.61
2:B:236:GLU:HG3	3:B:463:HOH:O	2.00	0.61
2:D:224:ARG:HG2	3:D:588:HOH:O	2.00	0.61
2:B:292:ARG:HG3	3:B:469:HOH:O	1.99	0.60
2:D:228:LEU:HD22	3:D:588:HOH:O	2.00	0.60
1:A:100:SER:HA	1:A:157:LEU:HD11	1.81	0.60
2:D:139:ARG:HD3	2:D:141:GLN:OE1	2.01	0.60
2:D:157:TYR:HD2	2:D:158:LEU:HD12	1.66	0.60
2:B:68:GLY:CA	2:B:116:VAL:HG13	2.32	0.60
1:A:53:TRP:CZ3	1:A:60:GLN:OE1	2.54	0.59
1:C:74:GLU:HG3	3:C:394:HOH:O	2.02	0.59
1:A:270:ARG:HD3	3:A:371:HOH:O	2.01	0.59
2:D:174:THR:O	2:D:178:ILE:HG12	2.02	0.59
1:A:134:ALA:C	1:A:136:PRO:HD3	2.23	0.59
2:D:59:HIS:ND1	3:D:528:HOH:O	2.31	0.59
2:B:16:HIS:NE2	2:B:280:ILE:HD11	2.18	0.59
1:C:252:ASN:ND2	1:C:270:ARG:HH11	1.98	0.59
2:D:45:ARG:NH2	2:D:140:PRO:HG3	2.18	0.58
1:A:58:ASP:HB2	1:A:106:HIS:O	2.04	0.58
2:D:9:PHE:CB	2:D:287:MET:O	2.50	0.58
2:B:181:THR:HG22	2:B:183:ARG:NH1	2.18	0.58
1:C:10:PRO:HB3	1:C:264:ALA:HB1	1.84	0.58
1:C:53:TRP:HH2	1:C:60:GLN:OE1	1.86	0.58
1:C:10:PRO:HG2	3:C:343:HOH:O	2.03	0.58
1:C:193:ILE:H	1:C:193:ILE:HD12	1.67	0.58
2:D:252:VAL:HG23	2:D:257:PHE:CB	2.34	0.58
2:B:202:PRO:HG2	2:B:205:PRO:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:ARG:O	2:B:228:LEU:HD13	2.05	0.57
2:B:22:ASN:N	2:B:23:PRO:HD3	2.19	0.57
2:B:226:ILE:HD11	2:D:39:TRP:CZ2	2.39	0.57
1:C:87:ARG:HE	1:C:133:ASP:HB3	1.68	0.57
2:D:9:PHE:CE1	2:D:51:MET:HE1	2.39	0.57
1:C:171:VAL:HG21	3:C:515:HOH:O	2.04	0.57
1:C:33:ARG:HG2	1:C:33:ARG:HH11	1.70	0.57
2:D:105:ALA:O	2:D:109:GLU:HB2	2.04	0.57
2:D:176:GLU:HA	2:D:176:GLU:OE1	2.04	0.57
1:A:62:LEU:HB3	3:A:307:HOH:O	2.05	0.56
1:A:10:PRO:HB2	1:A:12:THR:HG22	1.87	0.56
1:A:28:ALA:O	1:A:32:GLU:HG3	2.05	0.56
1:A:47:LEU:HD11	1:A:158:ALA:HB3	1.88	0.56
2:B:14:PRO:CG	2:B:17:LEU:HG	2.32	0.56
2:D:226:ILE:HD13	2:D:273:LEU:HD22	1.88	0.56
2:B:245:ILE:HD11	2:B:252:VAL:HG23	1.86	0.56
1:C:9:VAL:HG12	1:C:266:VAL:HG13	1.88	0.56
1:A:49:TYR:HB2	1:A:239:TRP:CD2	2.40	0.56
2:D:154:SER:HA	2:D:158:LEU:HD13	1.87	0.56
1:C:243:ALA:HB3	3:C:515:HOH:O	2.04	0.56
2:B:201:GLU:O	2:B:201:GLU:HG3	2.06	0.55
1:C:49:TYR:HB2	1:C:239:TRP:CE2	2.41	0.55
2:D:128:ASP:CB	3:D:476:HOH:O	2.51	0.55
2:B:196:TRP:HE1	2:B:248:ALA:HA	1.71	0.55
1:C:64:ARG:HB2	1:C:111:ASN:ND2	2.22	0.55
2:D:100:VAL:O	2:D:104:GLU:HG3	2.06	0.55
2:B:208:MET:HA	2:B:208:MET:HE2	1.89	0.55
2:D:161:LYS:HD3	2:D:161:LYS:N	2.22	0.55
2:B:179:ARG:HB3	2:B:299:LEU:HB2	1.88	0.55
2:B:164:MET:HE1	2:B:255:GLY:HA2	1.87	0.55
2:D:51:MET:HE2	2:D:186:VAL:HG11	1.87	0.55
1:A:22:PRO:HB2	3:A:327:HOH:O	2.06	0.55
2:D:56:LEU:HD12	2:D:186:VAL:HG22	1.88	0.55
2:B:82:VAL:HG22	2:B:91:ARG:HG2	1.89	0.54
2:D:22:ASN:N	2:D:23:PRO:HD3	2.22	0.54
1:A:10:PRO:HG2	3:A:408:HOH:O	2.07	0.54
2:D:6:ILE:HG21	2:D:51:MET:CG	2.36	0.54
2:D:85:ILE:HD12	2:D:85:ILE:N	2.22	0.54
2:D:61:PRO:HB3	2:D:254:SER:O	2.07	0.54
2:B:85:ILE:HD12	2:B:85:ILE:N	2.22	0.54
2:D:57:LEU:HG	2:D:147:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HD22	1:A:239:TRP:HZ2	1.72	0.54
1:A:195:ASN:HD22	1:A:195:ASN:N	2.05	0.54
2:B:52:LYS:N	2:B:53:PRO:HD3	2.23	0.54
1:C:195:ASN:HD22	1:C:198:ASP:CG	2.11	0.54
2:D:227:GLU:O	2:D:231:GLN:HG2	2.08	0.54
2:D:229:MET:HE2	2:D:287:MET:SD	2.48	0.54
2:B:92:TYR:OH	2:B:136:HIS:CD2	2.56	0.54
1:A:118:ASP:HA	3:A:484:HOH:O	2.07	0.53
1:C:271:LEU:HA	3:C:525:HOH:O	2.07	0.53
2:D:9:PHE:HE1	2:D:51:MET:HE1	1.71	0.53
1:A:53:TRP:HH2	1:A:110:VAL:HG21	1.72	0.53
1:A:65:PRO:HA	3:A:383:HOH:O	2.07	0.53
1:C:249:SER:O	1:C:250:GLY:O	2.25	0.53
2:D:226:ILE:HA	2:D:229:MET:HG3	1.91	0.53
1:A:99:SER:O	1:A:102:LEU:HB2	2.09	0.53
2:B:149:ILE:N	2:B:149:ILE:HD12	2.24	0.53
1:C:62:LEU:HD23	1:C:64:ARG:H	1.73	0.53
2:D:52:LYS:N	2:D:53:PRO:HD3	2.23	0.53
2:D:241:LEU:HB3	2:D:242:PRO:HD3	1.89	0.53
1:A:195:ASN:ND2	1:A:195:ASN:N	2.56	0.53
2:B:288:GLU:HG2	2:B:289:TRP:N	2.24	0.52
1:C:125:CYS:SG	1:C:137:LEU:HD11	2.48	0.52
2:D:211:GLU:HG3	2:D:278:THR:HG23	1.91	0.52
2:B:164:MET:CE	2:B:255:GLY:HA2	2.40	0.52
2:B:47:ARG:HH11	2:B:47:ARG:CG	2.22	0.52
2:B:219:TYR:CE2	2:D:208:MET:HG3	2.44	0.52
2:D:12:PRO:HB2	2:D:284:ASN:HD22	1.74	0.52
2:B:43:ARG:HB3	2:B:274:PHE:CD2	2.45	0.52
2:D:21:GLU:OE1	2:D:136:HIS:HE1	1.93	0.52
2:D:226:ILE:CD1	2:D:273:LEU:HD22	2.40	0.52
2:B:278:THR:HA	2:B:282:THR:O	2.09	0.52
2:B:55:VAL:HG22	2:B:56:LEU:N	2.25	0.52
2:D:139:ARG:NH1	2:D:141:GLN:HB2	2.17	0.52
1:C:225:ALA:HA	1:C:230:VAL:CG2	2.40	0.52
2:B:283:GLY:HA3	3:B:511:HOH:O	2.10	0.52
2:D:14:PRO:CG	2:D:17:LEU:HG	2.40	0.52
2:D:5:ILE:HD13	2:D:5:ILE:C	2.30	0.52
2:B:26:ASN:ND2	2:B:91:ARG:H	2.07	0.51
1:C:202:ASN:O	1:C:206:LEU:HB2	2.10	0.51
2:B:282:THR:HG22	2:B:284:ASN:HD21	1.76	0.51
2:B:15:PRO:O	2:B:18:VAL:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:TYR:HB2	1:C:239:TRP:CD2	2.45	0.51
1:A:77:TYR:CE1	2:B:120:MET:HA	2.45	0.51
2:B:111:ARG:HA	2:B:115:LEU:O	2.10	0.51
2:B:280:ILE:N	2:B:280:ILE:HD12	2.25	0.51
1:C:78:GLU:HG2	3:C:406:HOH:O	2.10	0.51
2:B:226:ILE:CD1	2:B:273:LEU:HD22	2.41	0.51
2:D:9:PHE:CD1	2:D:9:PHE:N	2.79	0.51
2:B:5:ILE:HG13	3:B:499:HOH:O	2.09	0.51
1:C:125:CYS:HA	1:C:130:ILE:CG1	2.41	0.51
2:D:5:ILE:HG23	2:D:5:ILE:O	2.11	0.51
2:B:5:ILE:HD11	2:B:178:ILE:HG13	1.93	0.51
1:A:187:ASP:HB3	1:A:190:GLU:HG2	1.92	0.50
1:A:49:TYR:HB2	1:A:239:TRP:CE2	2.47	0.50
2:B:85:ILE:HD11	3:B:475:HOH:O	2.11	0.50
1:C:20:GLU:H	1:C:20:GLU:CD	2.15	0.50
1:C:75:ASN:OD1	2:D:65:THR:HA	2.11	0.50
1:C:192:ARG:NH1	3:C:537:HOH:O	2.45	0.50
2:D:38:ARG:HG2	2:D:38:ARG:HH11	1.75	0.50
2:D:47:ARG:HD2	3:D:516:HOH:O	2.10	0.50
1:C:271:LEU:HG	3:C:525:HOH:O	2.10	0.50
2:D:158:LEU:N	2:D:158:LEU:HD12	2.27	0.50
2:D:154:SER:HB2	2:D:163:GLY:HA2	1.94	0.50
2:D:48:LEU:HB3	3:D:604:HOH:O	2.11	0.50
2:B:245:ILE:HD13	2:B:252:VAL:HG23	1.94	0.50
1:C:157:LEU:C	1:C:157:LEU:HD23	2.32	0.49
2:B:223:ILE:HG13	2:D:35:GLU:HG3	1.93	0.49
1:C:63:THR:O	1:C:90:THR:HG22	2.12	0.49
1:A:157:LEU:C	1:A:157:LEU:HD23	2.33	0.49
1:C:77:TYR:OH	2:D:70:HIS:HD2	1.95	0.49
1:A:53:TRP:HD1	1:A:118:ASP:OD1	1.94	0.49
3:A:570:HOH:O	2:B:154:SER:HB3	2.11	0.49
2:B:130:GLY:HA2	3:B:622:HOH:O	2.10	0.49
2:B:227:GLU:O	2:B:231:GLN:HB2	2.12	0.49
2:D:84:PRO:HG2	2:D:85:ILE:HD13	1.95	0.49
2:B:139:ARG:NH1	2:B:141:GLN:HE22	2.10	0.49
2:B:4:GLU:HG3	2:B:297:SER:HB2	1.94	0.49
1:C:18:LYS:HG3	1:C:20:GLU:OE2	2.14	0.48
2:D:51:MET:HB3	2:D:53:PRO:HG3	1.95	0.48
2:B:146:VAL:HG22	2:B:147:VAL:N	2.28	0.48
1:C:44:ASP:O	1:C:136:PRO:HD2	2.13	0.48
2:D:194:SER:HB3	2:D:222:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:HIS:O	2:D:200:GLU:HB2	2.13	0.48
2:D:252:VAL:CG2	2:D:257:PHE:HB3	2.42	0.48
2:B:233:LYS:HE2	3:B:553:HOH:O	2.14	0.48
2:D:39:TRP:O	2:D:42:GLU:HB2	2.14	0.48
1:C:18:LYS:HG2	1:C:21:VAL:HG23	1.96	0.48
1:A:143:ASN:HB3	1:A:146:HIS:CD2	2.48	0.47
1:A:47:LEU:HD11	1:A:158:ALA:CB	2.44	0.47
1:A:194:ALA:C	1:A:195:ASN:HD22	2.17	0.47
2:B:282:THR:HG22	2:B:284:ASN:ND2	2.30	0.47
2:D:13:HIS:HD2	2:D:190:SER:OG	1.98	0.47
2:D:164:MET:HB3	3:D:446:HOH:O	2.14	0.47
2:D:208:MET:HE2	2:D:208:MET:HA	1.95	0.47
1:A:152:GLU:HG2	1:A:238:HIS:O	2.14	0.47
1:C:183:ARG:NH2	2:D:154:SER:N	2.63	0.47
2:D:228:LEU:HB3	2:D:237:VAL:HG12	1.96	0.47
2:D:264:MET:O	2:D:267:PRO:HD3	2.14	0.47
2:B:56:LEU:O	2:B:146:VAL:HG23	2.15	0.47
2:B:48:LEU:HD11	2:B:53:PRO:HG2	1.97	0.47
2:D:225:MET:O	2:D:229:MET:HG2	2.13	0.47
2:D:226:ILE:O	2:D:230:ARG:HG3	2.14	0.47
2:B:57:LEU:HG	2:B:147:VAL:HB	1.96	0.47
2:D:233:LYS:HD3	2:D:236:GLU:OE2	2.15	0.47
2:B:179:ARG:HG3	2:B:180:LYS:H	1.79	0.47
2:D:184:LYS:N	2:D:184:LYS:HD2	2.30	0.47
2:B:267:PRO:C	2:B:269:LEU:H	2.17	0.47
2:B:2:GLN:HE21	2:B:300:GLY:HA2	1.80	0.47
1:C:225:ALA:HA	1:C:230:VAL:HB	1.96	0.47
2:D:202:PRO:O	2:D:203:THR:HB	2.15	0.47
2:B:63:TRP:CZ3	2:B:72:LEU:HD13	2.50	0.46
2:D:256:ALA:C	3:D:403:HOH:O	2.53	0.46
1:A:117:ILE:HG22	1:A:122:ILE:HG13	1.97	0.46
2:B:61:PRO:HB3	2:B:254:SER:OG	2.14	0.46
1:A:225:ALA:HA	1:A:230:VAL:HB	1.97	0.46
1:A:244:LEU:HD22	1:A:271:LEU:HD22	1.96	0.46
2:B:226:ILE:HD12	2:B:273:LEU:HD22	1.96	0.46
1:A:271:LEU:HD13	3:A:577:HOH:O	2.15	0.46
2:B:35:GLU:HG3	2:D:223:ILE:CD1	2.46	0.46
2:B:61:PRO:HB3	2:B:254:SER:CB	2.45	0.46
1:C:58:ASP:OD1	2:D:200:GLU:HG3	2.15	0.46
2:D:85:ILE:N	2:D:85:ILE:CD1	2.78	0.46
2:B:121:ARG:HG3	2:B:121:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLY:O	1:A:38:LEU:HB3	2.16	0.46
1:A:136:PRO:HG2	3:A:526:HOH:O	2.16	0.45
2:B:76:GLU:HB3	3:B:650:HOH:O	2.15	0.45
1:C:87:ARG:HE	1:C:133:ASP:CB	2.29	0.45
1:C:205:VAL:HG11	1:C:224:TYR:CD2	2.51	0.45
1:A:201:TRP:O	1:A:205:VAL:HG13	2.17	0.45
2:B:68:GLY:HA3	2:B:116:VAL:HG22	1.99	0.45
2:B:164:MET:HE3	2:B:164:MET:HA	1.97	0.45
2:B:228:LEU:HB3	2:B:237:VAL:HG12	1.99	0.45
2:D:160:THR:O	2:D:164:MET:HG2	2.16	0.45
1:C:33:ARG:NH1	1:C:33:ARG:HG2	2.31	0.45
2:D:59:HIS:HE1	2:D:255:GLY:HA3	1.82	0.45
1:C:249:SER:O	1:C:270:ARG:O	2.35	0.45
2:B:164:MET:HG2	3:B:620:HOH:O	2.16	0.45
2:D:41:TYR:CE1	2:D:137:LEU:HG	2.52	0.45
2:D:245:ILE:HD13	2:D:253:LYS:HB2	1.98	0.45
2:D:229:MET:CE	2:D:287:MET:SD	3.05	0.45
1:A:38:LEU:HD13	1:A:43:PRO:HG3	1.99	0.45
1:C:193:ILE:N	1:C:193:ILE:HD12	2.31	0.45
2:D:55:VAL:HG23	2:D:145:PRO:O	2.16	0.45
2:D:42:GLU:O	2:D:46:GLU:HG3	2.17	0.45
1:A:155:ALA:HB2	1:A:239:TRP:CE3	2.52	0.45
2:D:157:TYR:CD2	2:D:158:LEU:HD12	2.50	0.45
2:B:279:VAL:HG13	2:B:279:VAL:O	2.17	0.44
2:D:63:TRP:CZ3	2:D:72:LEU:HD13	2.52	0.44
2:B:26:ASN:HD21	2:B:91:ARG:N	2.12	0.44
2:B:284:ASN:N	2:B:284:ASN:HD22	2.10	0.44
2:B:35:GLU:H	2:B:35:GLU:CD	2.20	0.44
1:C:77:TYR:CE1	2:D:120:MET:HA	2.52	0.44
2:D:156:TYR:OH	2:D:254:SER:HA	2.17	0.44
1:C:54:LEU:HD22	1:C:144:LEU:CD2	2.41	0.44
1:C:77:TYR:OH	2:D:70:HIS:CD2	2.71	0.44
2:D:4:GLU:HG3	2:D:297:SER:O	2.17	0.44
2:B:16:HIS:CD2	2:B:280:ILE:HD11	2.52	0.44
1:A:77:TYR:HE2	2:B:70:HIS:HD2	1.66	0.44
2:D:53:PRO:HB3	2:D:186:VAL:HG13	1.99	0.44
2:D:201:GLU:HB2	2:D:202:PRO:HD2	2.00	0.44
1:C:59:GLN:HG2	1:C:146:HIS:NE2	2.32	0.44
2:D:72:LEU:HD22	2:D:148:GLY:HA3	1.99	0.44
2:D:55:VAL:HG22	2:D:56:LEU:N	2.33	0.44
2:B:47:ARG:NH1	2:B:47:ARG:CG	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:LEU:H	1:C:271:LEU:CD1	2.30	0.44
2:B:179:ARG:HB3	2:B:299:LEU:CB	2.48	0.44
2:B:74:VAL:O	2:B:98:VAL:HB	2.18	0.44
1:C:212:GLY:O	1:C:214:VAL:N	2.48	0.44
2:D:219:TYR:O	2:D:223:ILE:HG12	2.17	0.44
2:D:214:ALA:HB2	2:D:281:GLY:HA3	2.00	0.44
1:A:49:TYR:OH	1:A:235:LYS:HE3	2.17	0.43
1:A:94:GLU:HG3	3:A:445:HOH:O	2.18	0.43
2:B:179:ARG:NH2	3:B:418:HOH:O	2.51	0.43
1:C:149:GLU:HG2	3:C:547:HOH:O	2.18	0.43
2:B:219:TYR:O	2:B:223:ILE:HG12	2.18	0.43
2:B:41:TYR:O	2:B:45:ARG:HG3	2.17	0.43
1:C:51:THR:HG21	1:C:231:ASP:OD1	2.17	0.43
1:C:237:LEU:HD13	1:C:237:LEU:C	2.38	0.43
2:D:84:PRO:HG2	2:D:85:ILE:CD1	2.48	0.43
2:B:171:GLY:HA3	2:B:262:ALA:HB3	2.00	0.43
2:B:223:ILE:CG2	2:D:35:GLU:HG3	2.48	0.43
2:D:212:TYR:CA	2:D:278:THR:HG21	2.46	0.43
1:A:134:ALA:O	1:A:136:PRO:HD3	2.19	0.43
2:B:126:ARG:HG3	3:B:540:HOH:O	2.18	0.43
2:B:35:GLU:HG2	2:D:219:TYR:OH	2.17	0.43
1:C:131:GLY:HA2	1:C:137:LEU:HG	2.00	0.43
1:C:87:ARG:NH2	3:C:445:HOH:O	2.52	0.43
2:D:15:PRO:HB2	2:D:90:PHE:HB2	2.00	0.43
2:D:6:ILE:O	2:D:291:LEU:HB2	2.18	0.43
2:B:251:GLU:HG2	2:B:251:GLU:O	2.18	0.43
2:B:260:MET:O	2:B:264:MET:HG3	2.18	0.43
1:C:183:ARG:HH22	2:D:153:ASN:CB	2.31	0.43
1:A:115:PHE:HA	1:A:116:PRO:HD3	1.71	0.43
1:A:31:THR:HG22	1:A:127:LEU:HB3	1.99	0.43
2:B:226:ILE:HA	2:B:229:MET:CE	2.48	0.43
1:C:210:GLU:O	1:C:250:GLY:HA2	2.18	0.43
1:A:216:ALA:O	1:A:219:GLU:HG3	2.19	0.43
2:B:179:ARG:HG3	2:B:180:LYS:N	2.33	0.43
1:C:49:TYR:OH	1:C:235:LYS:HE2	2.18	0.43
2:D:41:TYR:CE2	2:D:137:LEU:HB3	2.53	0.43
2:D:256:ALA:N	3:D:528:HOH:O	2.45	0.43
1:C:244:LEU:HG	3:C:515:HOH:O	2.18	0.42
2:D:229:MET:HG2	2:D:229:MET:H	1.60	0.42
1:A:244:LEU:CD2	1:A:271:LEU:HD22	2.49	0.42
2:B:223:ILE:CG1	2:D:35:GLU:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:PRO:HG3	3:B:453:HOH:O	2.19	0.42
2:B:26:ASN:HA	2:B:26:ASN:HD22	1.67	0.42
1:C:100:SER:CA	1:C:157:LEU:HD11	2.37	0.42
2:D:139:ARG:HH11	2:D:141:GLN:CB	2.19	0.42
2:D:59:HIS:CE1	2:D:256:ALA:H	2.37	0.42
2:B:216:MET:O	2:B:220:GLN:HG3	2.19	0.42
2:B:25:GLN:N	2:B:25:GLN:HE21	2.08	0.42
1:C:17:LEU:HD13	1:C:82:LEU:HD21	2.02	0.42
2:D:12:PRO:HB2	2:D:14:PRO:HD3	2.01	0.42
2:D:206:GLU:O	2:D:208:MET:N	2.53	0.42
2:D:96:LEU:C	2:D:96:LEU:HD12	2.39	0.42
2:B:98:VAL:HA	2:B:146:VAL:O	2.19	0.42
2:B:204:ILE:O	2:B:204:ILE:HG23	2.19	0.42
2:B:280:ILE:O	2:B:280:ILE:CG2	2.65	0.42
2:D:38:ARG:NH1	2:D:38:ARG:HG2	2.34	0.42
2:B:55:VAL:HG11	2:B:102:LEU:CD2	2.50	0.42
1:C:271:LEU:N	1:C:271:LEU:CD1	2.82	0.42
2:D:81:SER:OG	2:D:129:TYR:HA	2.20	0.42
2:D:251:GLU:HG2	2:D:254:SER:HB2	2.01	0.42
1:C:201:TRP:CZ3	1:C:204:ARG:HD2	2.55	0.42
2:D:157:TYR:HD2	2:D:158:LEU:CD1	2.33	0.42
1:A:189:ARG:HG2	3:A:439:HOH:O	2.19	0.42
1:A:224:TYR:CE2	1:A:230:VAL:HG21	2.55	0.42
1:A:31:THR:CG2	1:A:127:LEU:HB3	2.50	0.42
2:B:208:MET:CA	2:B:208:MET:HE2	2.50	0.42
2:B:2:GLN:CB	2:B:298:MET:HE3	2.50	0.42
2:D:22:ASN:OD1	2:D:29:ARG:HA	2.20	0.42
2:B:109:GLU:OE2	2:B:176:GLU:HG2	2.20	0.42
1:C:187:ASP:HB3	1:C:190:GLU:HG3	2.01	0.42
1:C:237:LEU:HD13	1:C:237:LEU:O	2.20	0.42
2:D:216:MET:O	2:D:220:GLN:HG3	2.20	0.42
2:D:61:PRO:CB	2:D:254:SER:HB3	2.45	0.42
2:B:154:SER:HB2	2:B:163:GLY:HA2	2.01	0.42
2:B:276:TYR:HE1	3:B:511:HOH:O	2.02	0.42
2:B:84:PRO:HG2	2:B:85:ILE:CD1	2.47	0.42
2:B:74:VAL:CG2	2:B:77:LEU:HG	2.49	0.41
2:D:226:ILE:HD12	2:D:226:ILE:C	2.40	0.41
2:D:231:GLN:HA	2:D:231:GLN:HE21	1.85	0.41
1:A:64:ARG:HB2	1:A:111:ASN:OD1	2.20	0.41
1:C:152:GLU:HG2	1:C:238:HIS:O	2.20	0.41
2:D:17:LEU:HD11	2:D:37:LEU:CB	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:GLU:CG	2:D:254:SER:HB2	2.50	0.41
1:A:226:LYS:HG2	3:A:622:HOH:O	2.19	0.41
2:D:154:SER:OG	2:D:155:PRO:HD3	2.20	0.41
2:D:159:ASN:OD1	2:D:161:LYS:HG2	2.20	0.41
1:A:87:ARG:HG2	1:A:131:GLY:O	2.21	0.41
2:B:241:LEU:HB3	2:B:242:PRO:HD3	2.03	0.41
2:D:256:ALA:O	3:D:408:HOH:O	2.22	0.41
2:D:267:PRO:C	2:D:269:LEU:H	2.23	0.41
1:A:116:PRO:HG3	3:B:401:HOH:O	2.20	0.41
1:A:10:PRO:HB3	1:A:264:ALA:HB1	2.01	0.41
1:A:68:GLU:HB2	3:A:436:HOH:O	2.21	0.41
2:D:4:GLU:HG3	2:D:297:SER:HB2	2.02	0.41
1:A:110:VAL:HG23	1:A:110:VAL:O	2.21	0.41
1:C:58:ASP:OD2	2:D:200:GLU:HG3	2.21	0.41
2:D:92:TYR:OH	2:D:136:HIS:CD2	2.68	0.41
2:B:236:GLU:HB3	3:B:559:HOH:O	2.20	0.41
1:C:6:ALA:C	1:C:7:PHE:CD1	2.94	0.41
2:B:46:GLU:HB2	3:B:586:HOH:O	2.20	0.41
1:C:84:TYR:HB2	1:C:86:ILE:HD12	2.02	0.41
1:A:26:GLN:NE2	3:A:497:HOH:O	2.53	0.41
2:B:12:PRO:O	2:B:14:PRO:HD2	2.21	0.41
2:B:55:VAL:CG1	2:B:185:ALA:HB2	2.51	0.41
2:B:19:TYR:CE1	2:B:30:SER:HB3	2.55	0.41
1:A:253:VAL:HG11	3:A:359:HOH:O	2.20	0.41
1:A:62:LEU:HD22	1:A:64:ARG:H	1.86	0.41
1:C:100:SER:N	1:C:101:PRO:HD2	2.36	0.41
1:C:53:TRP:CH2	1:C:60:GLN:OE1	2.72	0.40
2:D:128:ASP:HB2	2:D:131:THR:H	1.85	0.40
1:C:61:TRP:O	1:C:63:THR:HG23	2.22	0.40
2:D:223:ILE:O	2:D:227:GLU:HB2	2.20	0.40
2:D:239:LYS:HA	2:D:239:LYS:HD3	1.92	0.40
2:D:193:LEU:O	2:D:250:ALA:HA	2.21	0.40
2:B:226:ILE:HG13	2:B:227:GLU:N	2.36	0.40
2:B:228:LEU:CB	2:B:237:VAL:HG12	2.52	0.40
1:A:77:TYR:CE2	2:B:70:HIS:HD2	2.39	0.40
2:D:231:GLN:HA	2:D:231:GLN:NE2	2.36	0.40
2:B:195:HIS:HB3	2:B:249:PHE:CD2	2.56	0.40
2:B:85:ILE:CD1	3:B:475:HOH:O	2.69	0.40
2:B:97:ASN:O	2:B:146:VAL:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	268/271 (99%)	254 (95%)	13 (5%)	1 (0%)	34	48
1	C	268/271 (99%)	254 (95%)	12 (4%)	2 (1%)	22	32
2	B	302/312 (97%)	285 (94%)	16 (5%)	1 (0%)	41	55
2	D	298/312 (96%)	278 (93%)	15 (5%)	5 (2%)	9	11
All	All	1136/1166 (97%)	1071 (94%)	56 (5%)	9 (1%)	19	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	250	GLY
2	D	254	SER
2	B	203	THR
2	D	2	GLN
2	D	207	ASP
1	A	22	PRO
2	D	6	ILE
2	D	280	ILE
1	C	22	PRO

5.3.2 Protein sidechains

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	212/213 (100%)	188 (89%)	24 (11%)	6	8
1	C	212/213 (100%)	191 (90%)	21 (10%)	8	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	253/258 (98%)	235 (93%)	18 (7%)	14 23
2	D	251/258 (97%)	229 (91%)	22 (9%)	10 15
All	All	928/942 (98%)	843 (91%)	85 (9%)	9 13

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	14	LEU
1	A	17	LEU
1	A	38	LEU
1	A	47	LEU
1	A	53	TRP
1	A	62	LEU
1	A	87	ARG
1	A	92	LEU
1	A	102	LEU
1	A	127	LEU
1	A	144	LEU
1	A	154	LEU
1	A	157	LEU
1	A	160	ASP
1	A	195	ASN
1	A	201	TRP
1	A	205	VAL
1	A	206	LEU
1	A	207	LYS
1	A	208	LEU
1	A	219	GLU
1	A	234	PHE
1	A	260	TYR
2	B	18	VAL
2	B	25	GLN
2	B	26	ASN
2	B	31	GLN
2	B	38	ARG
2	B	41	TYR
2	B	47	ARG
2	B	70	HIS
2	B	72	LEU
2	B	76	GLU

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Mol	Chain	Res	Type
2	B	96	LEU
2	B	116	VAL
2	B	137	LEU
2	B	138	ILE
2	B	153	ASN
2	B	164	MET
2	B	179	ARG
2	B	204	ILE
1	C	12	THR
1	C	14	LEU
1	C	17	LEU
1	C	47	LEU
1	C	53	TRP
1	C	59	GLN
1	C	64	ARG
1	C	92	LEU
1	C	102	LEU
1	C	111	ASN
1	C	127	LEU
1	C	154	LEU
1	C	157	LEU
1	C	171	VAL
1	C	181	LEU
1	C	196	GLU
1	C	201	TRP
1	C	221	MET
1	C	226	LYS
1	C	234	PHE
1	C	260	TYR
2	D	5	ILE
2	D	9	PHE
2	D	17	LEU
2	D	18	VAL
2	D	25	GLN
2	D	35	GLU
2	D	38	ARG
2	D	41	TYR
2	D	51	MET
2	D	72	LEU
2	D	74	VAL
2	D	116	VAL
2	D	137	LEU

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Mol	Chain	Res	Type
2	D	139	ARG
2	D	153	ASN
2	D	176	GLU
2	D	184	LYS
2	D	201	GLU
2	D	226	ILE
2	D	229	MET
2	D	237	VAL
2	D	272	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	60	GLN
1	A	71	HIS
1	A	146	HIS
1	A	195	ASN
2	B	2	GLN
2	B	25	GLN
2	B	26	ASN
2	B	62	HIS
2	B	70	HIS
2	B	136	HIS
2	B	153	ASN
2	B	265	GLN
2	B	284	ASN
1	C	71	HIS
1	C	106	HIS
1	C	111	ASN
1	C	195	ASN
1	C	238	HIS
1	C	252	ASN
2	D	13	HIS
2	D	25	GLN
2	D	70	HIS
2	D	136	HIS
2	D	153	ASN
2	D	197	HIS
2	D	220	GLN
2	D	231	GLN
2	D	265	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	270/271 (99%)	-0.72	0	100	100	7, 18, 30, 38	0
1	C	270/271 (99%)	-0.53	0	100	100	12, 22, 34, 40	0
2	B	304/312 (97%)	-0.38	2 (0%)	87	86	13, 25, 43, 72	0
2	D	300/312 (96%)	-0.31	4 (1%)	77	75	12, 24, 43, 72	0
All	All	1144/1166 (98%)	-0.48	6 (0%)	91	89	7, 23, 38, 72	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	203	THR	4.1
2	D	254	SER	3.0
2	D	200	GLU	2.6
2	D	202	PRO	2.2
2	B	201	GLU	2.1
2	B	199	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.