Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 03:29 pm GMT

PDB ID	:	5FO9
Title	:	Crystal Structure of Human Complement C3b in Complex with CR1 (CCP15-17)
Authors	:	Forneris, F.; Wu, J.; Xue, X.; Gros, P.
Deposited on	:	2015-11-18
Resolution	:	3.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

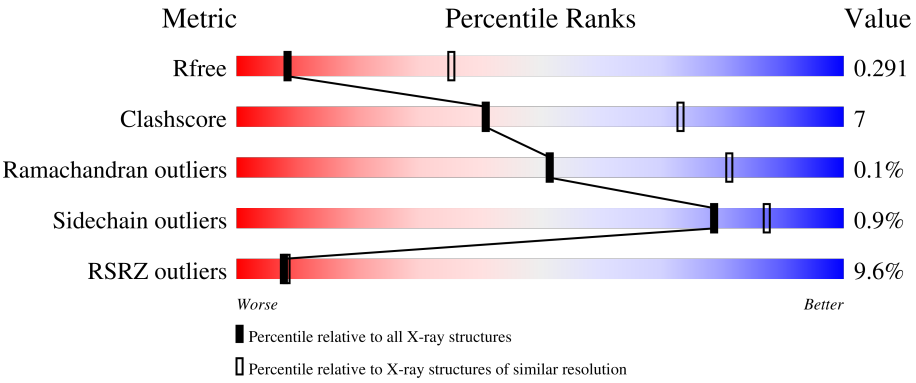
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	645	3% 78% 21% ·
1	D	645	4% 80% 19%
2	B	915	13% 83% 15% ·
2	E	915	8% 80% 18% ·
3	C	196	23% 79% 19% ··

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Mol	Chain	Length	Quality of chain
3	F	196	28% 81% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1063	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27406 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5007	3187	848	957	15			
1	D	642	Total	C	N	O	S	0	0	0
			5007	3187	848	957	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	903	Total	C	N	O	S	0	0	0
			7208	4568	1212	1391	37			
2	E	903	Total	C	N	O	S	0	0	0
			7208	4568	1212	1391	37			

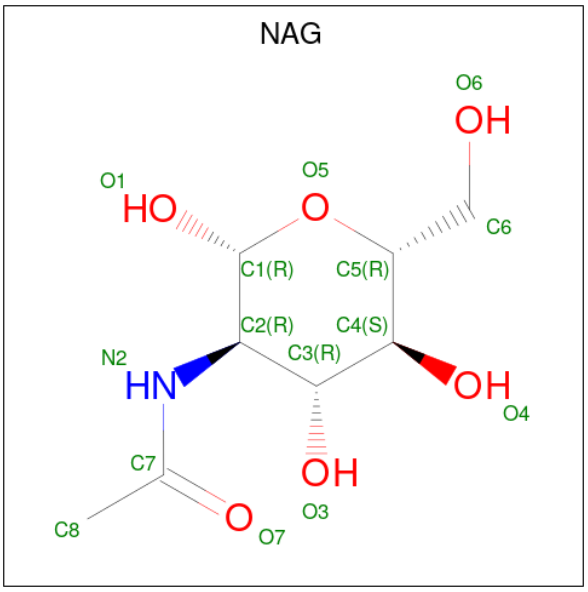
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	SEE REMARK 999	UNP P01024
E	1013	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called COMPLEMENT RECEPTOR TYPE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	194	Total	C	N	O	S	0	0	1
			1474	925	258	278	13			
3	F	194	Total	C	N	O	S	0	0	1
			1474	925	258	278	13			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



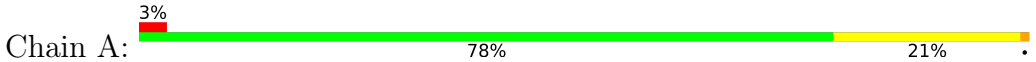
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

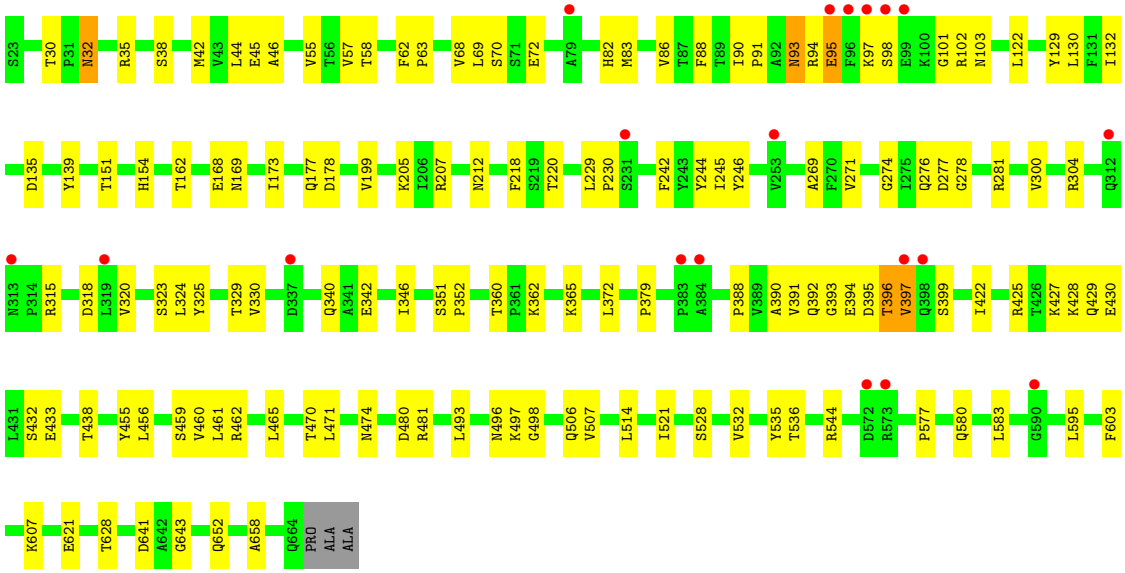
3 Residue-property plots (i)

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: COMPLEMENT C3 BETA CHAIN

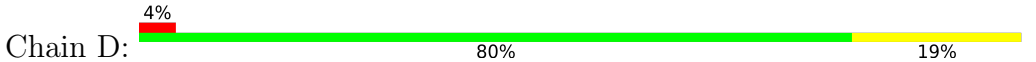
Chain A:

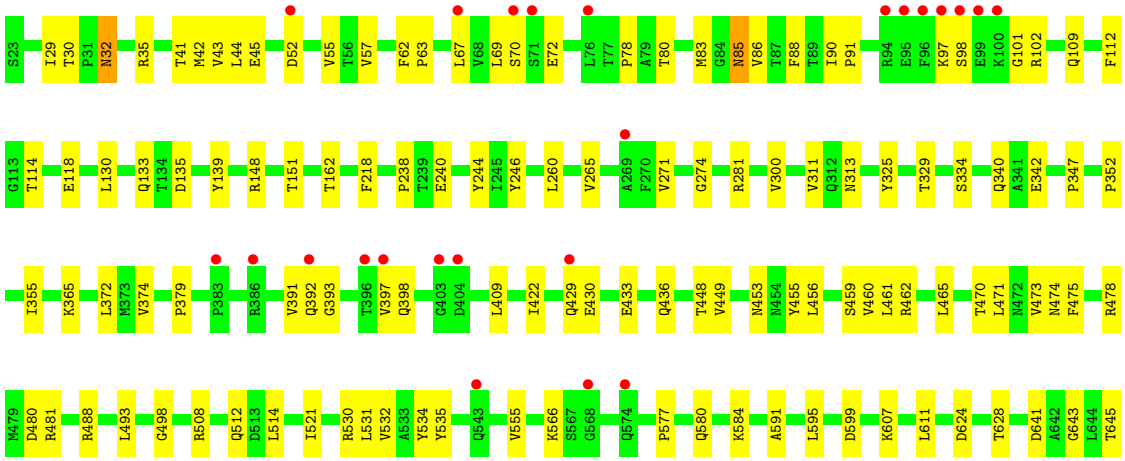


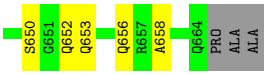


• Molecule 1: COMPLEMENT C3 BETA CHAIN

Chain D:

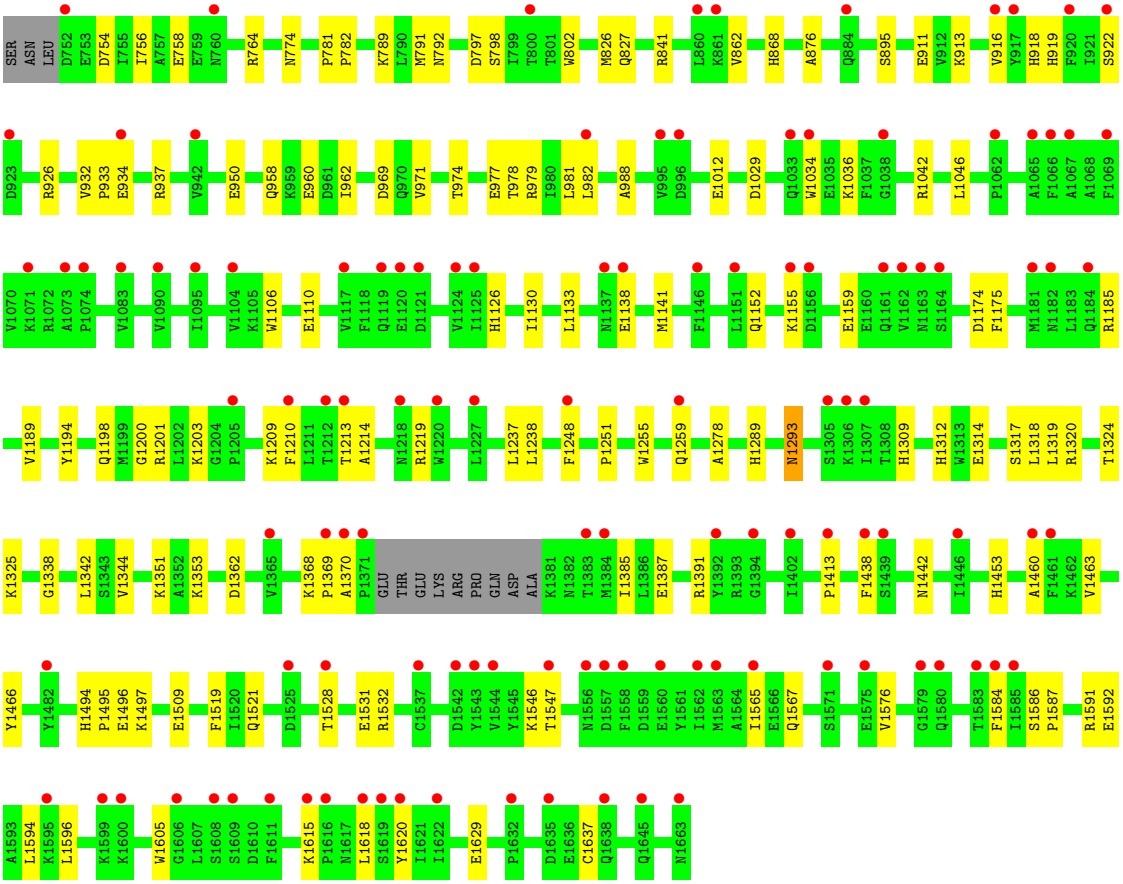






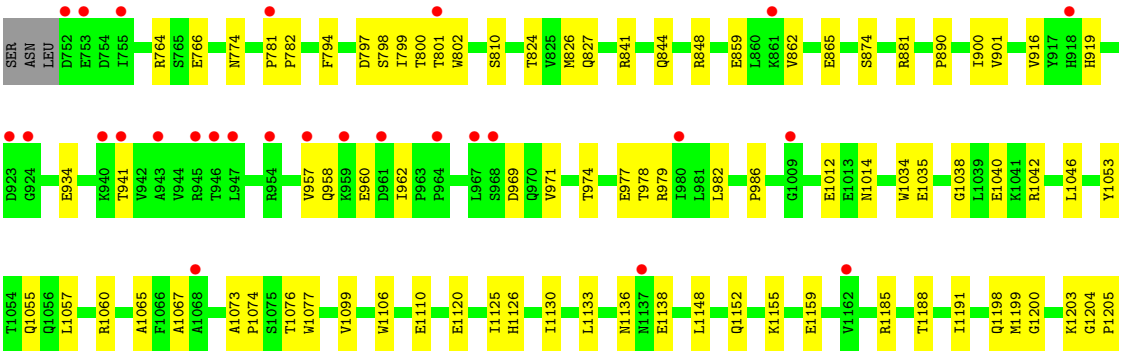
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

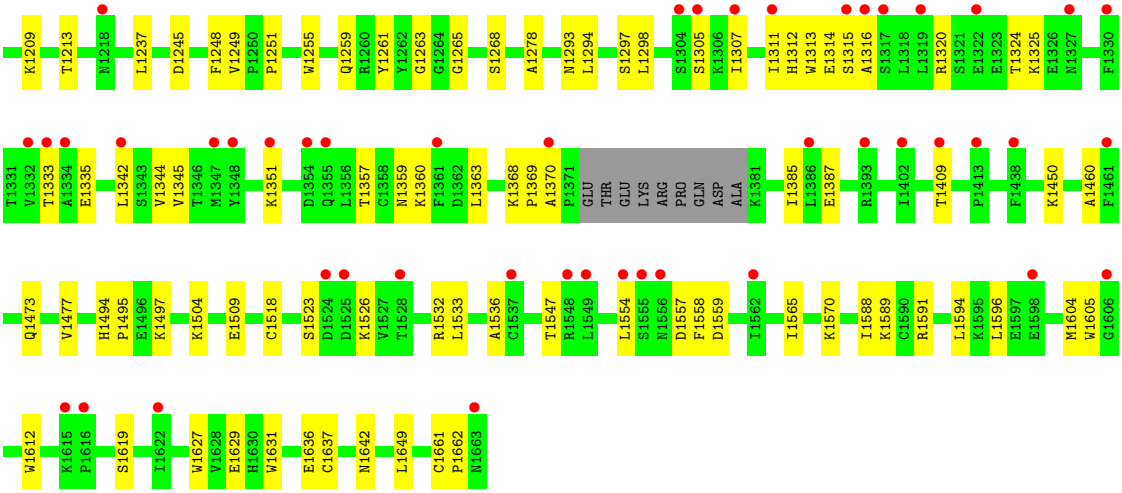
Chain B:



• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

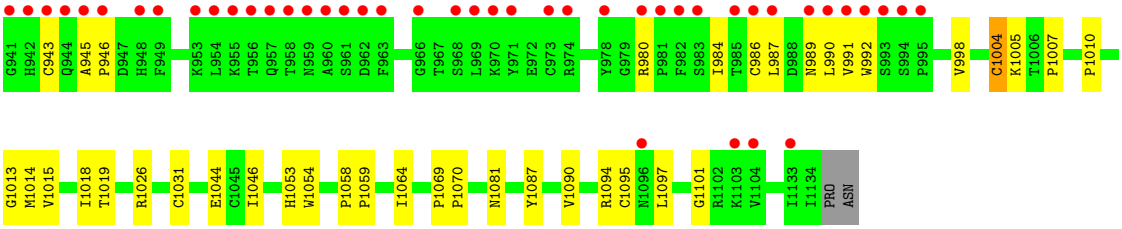
Chain E:





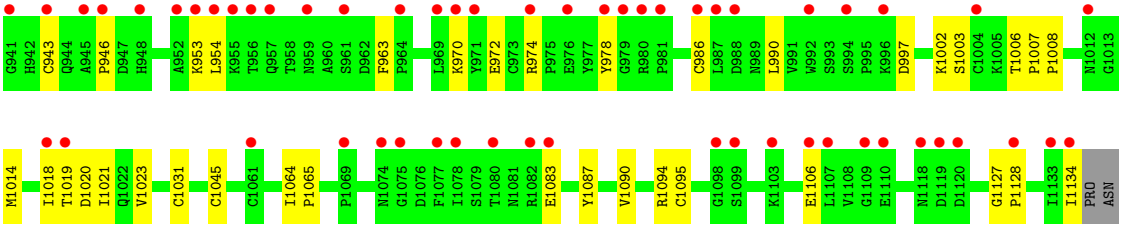
• Molecule 3: COMPLEMENT RECEPTOR TYPE 1

Chain C:



• Molecule 3: COMPLEMENT RECEPTOR TYPE 1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	104.32Å 113.71Å 138.52Å 82.74° 71.77° 80.95°	Depositor
Resolution (Å)	60.15 – 3.30 60.15 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (60.15-3.30) 93.2 (60.15-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.251 , 0.291 0.253 , 0.291	Depositor DCC
R_{free} test set	4424 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	62.8	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 85.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	27406	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.27% 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: NAG

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	0.24	0/5108	0.47	0/6940
1	D	0.23	0/5108	0.46	0/6940
2	B	0.23	0/7352	0.44	0/9955
2	E	0.23	0/7352	0.43	0/9955
3	C	0.27	0/1515	0.51	0/2066
3	F	0.27	0/1515	0.55	0/2066
All	All	0.24	0/27950	0.46	0/37922

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	5007	0	5064	86	0
1	D	5007	0	5063	79	0
2	B	7208	0	7128	85	0
2	E	7208	0	7130	120	0
3	C	1474	0	1407	23	0
3	F	1474	0	1407	23	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	14	0	12	1	0
All	All	27406	0	27224	388	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 7.

All (388) 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:E:1554:LEU:CD2	2:E:1591:ARG:HH11	1.39	1.33
2:E:1554:LEU:CD1	2:E:1591:ARG:HH12	1.49	1.24
2:E:1559:ASP:OD2	2:E:1591:ARG:CG	1.90	1.19
2:E:1554:LEU:CD1	2:E:1591:ARG:NH1	2.05	1.19
2:E:1554:LEU:HD13	2:E:1591:ARG:NH1	1.57	1.17
2:E:1559:ASP:CG	2:E:1591:ARG:HD3	1.68	1.14
2:E:1554:LEU:HD22	2:E:1591:ARG:HH11	1.01	1.07
2:E:1554:LEU:CD2	2:E:1591:ARG:NH1	2.17	1.07
2:E:1559:ASP:OD2	2:E:1591:ARG:HG3	1.59	1.02
2:E:1554:LEU:HD22	2:E:1591:ARG:NH1	1.74	1.02
2:E:1559:ASP:OD1	2:E:1591:ARG:HD3	1.64	0.94
2:E:1554:LEU:HD13	2:E:1591:ARG:HH12	0.76	0.91
2:E:1559:ASP:CG	2:E:1591:ARG:CD	2.44	0.85
2:E:1559:ASP:OD2	2:E:1591:ARG:CD	2.28	0.82
2:E:1559:ASP:OD2	2:E:1591:ARG:HG2	1.82	0.80
1:A:365:LYS:HD3	1:A:455:TYR:HB3	1.63	0.80
1:A:461:LEU:HB2	1:D:461:LEU:HD12	1.69	0.75
2:E:1554:LEU:HD21	2:E:1591:ARG:HH11	1.45	0.75
2:E:1559:ASP:OD2	2:E:1591:ARG:HD3	1.89	0.73
1:A:168:GLU:HB2	1:A:205:LYS:HG3	1.72	0.72
2:E:1554:LEU:CG	2:E:1591:ARG:NH1	2.52	0.72
1:A:462:ARG:NH2	1:A:470:THR:O	2.18	0.71
1:D:41:THR:HG21	4:D:1063:NAG:H82	1.73	0.70
1:D:260:LEU:HB3	2:E:800:THR:HG23	1.74	0.70
1:A:456:LEU:HB2	1:A:535:TYR:HE2	1.57	0.69
1:D:462:ARG:NH2	1:D:470:THR:O	2.23	0.69
2:E:774:ASN:ND2	3:F:1014:MET:SD	2.65	0.69
2:B:1594:LEU:HB3	2:B:1596:LEU:HG	1.75	0.68
1:A:432:SER:OG	1:A:433:GLU:N	2.27	0.68
2:E:1554:LEU:HD11	2:E:1591:ARG:NH1	2.06	0.68
1:A:480:ASP:HA	1:D:481:ARG:HH22	1.58	0.67
2:B:1155:LYS:O	2:B:1159:GLU:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1294:LEU:HB2	2:E:1311:ILE:HB	1.78	0.66
2:B:841:ARG:HH12	2:B:1509:GLU:HB3	1.59	0.66
2:B:862:VAL:HG22	2:B:916:VAL:HG12	1.76	0.66
1:A:460:VAL:HG13	1:A:471:LEU:HD11	1.79	0.65
3:C:1004:CYS:O	3:C:1054:TRP:NE1	2.29	0.64
2:B:774:ASN:ND2	3:C:1014:MET:SD	2.70	0.64
2:E:764:ARG:HB3	2:E:797:ASP:HB3	1.80	0.64
2:E:1594:LEU:HB3	2:E:1596:LEU:HG	1.80	0.64
2:B:1528:THR:H	2:B:1531:GLU:HG3	1.63	0.63
1:A:30:THR:HG22	1:A:42:MET:HG3	1.80	0.63
2:E:1298:LEU:HB2	2:E:1307:ILE:HB	1.81	0.63
1:A:103:ASN:ND2	1:A:658:ALA:O	2.31	0.62
1:A:135:ASP:OD1	1:A:139:TYR:OH	2.12	0.62
1:A:394:GLU:HG3	1:A:397:VAL:HG12	1.82	0.62
2:E:1312:HIS:N	2:E:1315:SER:OG	2.31	0.62
1:D:271:VAL:HG21	1:D:300:VAL:HG11	1.81	0.61
3:C:984:ILE:HD12	3:C:992:TRP:HB3	1.81	0.61
1:A:465:LEU:HD11	1:A:521:ILE:HG13	1.82	0.60
2:E:1200:GLY:O	2:E:1203:LYS:NZ	2.33	0.60
1:A:315:ARG:NH2	1:A:318:ASP:OD1	2.34	0.60
2:B:754:ASP:H	3:C:980:ARG:HH12	1.49	0.60
2:B:1012:GLU:OE1	2:B:1126:HIS:ND1	2.25	0.60
2:E:1636:GLU:O	2:E:1642:ASN:ND2	2.35	0.59
2:E:1532:ARG:NH2	2:E:1629:GLU:OE2	2.33	0.59
1:D:448:THR:HG21	1:D:453:ASN:H	1.68	0.59
2:E:794:PHE:HE2	3:F:1006:THR:HG23	1.67	0.59
2:B:1494:HIS:HB3	2:B:1497:LYS:HB2	1.84	0.59
2:B:950:GLU:OE2	2:B:1338:GLY:N	2.31	0.59
1:A:177:GLN:NE2	2:B:1319:LEU:O	2.36	0.58
2:B:1362:ASP:OD2	2:B:1391:ARG:NH2	2.36	0.58
1:D:162:THR:HG23	3:F:1090:VAL:HG11	1.83	0.58
1:D:465:LEU:HD21	1:D:521:ILE:HG21	1.85	0.58
1:A:245:ILE:O	1:A:304:ARG:NE	2.28	0.58
1:A:162:THR:HG23	3:C:1090:VAL:HG11	1.84	0.58
1:D:456:LEU:HB2	1:D:535:TYR:HE2	1.69	0.57
2:B:1130:ILE:HD12	2:B:1133:LEU:HB2	1.87	0.57
1:A:178:ASP:OD1	3:C:1081:ASN:ND2	2.38	0.57
2:B:1130:ILE:HB	2:B:1133:LEU:HD12	1.86	0.57
2:E:1588:ILE:O	2:E:1589:LYS:HG2	2.05	0.56
2:E:1557:ASP:N	2:E:1557:ASP:OD1	2.38	0.56
1:A:97:LYS:HB3	1:A:98:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1010:PRO:HG2	3:C:1013:GLY:HA3	1.87	0.56
1:D:45:GLU:HG2	1:D:83:MET:HG3	1.87	0.56
1:D:30:THR:HG22	1:D:42:MET:HG3	1.87	0.56
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.87	0.55
2:E:1612:TRP:HB3	2:E:1619:SER:HB2	1.89	0.55
3:C:1026:ARG:HG2	3:C:1044:GLU:HG2	1.87	0.55
1:A:94:ARG:HB2	1:A:212:ASN:HA	1.87	0.54
3:C:1004:CYS:HB3	3:C:1054:TRP:CE2	2.42	0.54
1:A:57:VAL:HB	1:A:72:GLU:HB2	1.87	0.54
2:B:1189:VAL:HG12	2:B:1210:PHE:HD1	1.73	0.54
2:B:1370:ALA:HB2	2:B:1385:ILE:HG13	1.89	0.54
1:D:97:LYS:HE2	2:E:1313:TRP:HZ3	1.73	0.54
2:B:1141:MET:HG2	2:B:1175:PHE:HE2	1.74	0.54
1:A:528:SER:OG	1:A:621:GLU:OE2	2.25	0.53
1:D:397:VAL:O	1:D:398:GLN:HG2	2.07	0.53
3:C:1004:CYS:O	3:C:1005:LYS:HG2	2.07	0.53
2:E:986:PRO:HG3	2:E:1316:ALA:HB1	1.90	0.53
2:E:1067:ALA:HB2	2:E:1074:PRO:HA	1.90	0.53
2:B:1494:HIS:O	2:B:1496:GLU:HA	2.09	0.53
2:B:962:ILE:HD13	2:B:1344:VAL:HG21	1.90	0.53
1:D:98:SER:OG	1:D:101:GLY:O	2.23	0.53
3:F:953:LYS:N	3:F:972:GLU:O	2.22	0.53
1:A:57:VAL:HG21	1:A:86:VAL:HG21	1.91	0.53
2:B:1615:LYS:HG2	2:B:1618:LEU:HD11	1.90	0.52
2:E:957:VAL:HG22	2:E:1335:GLU:HG3	1.91	0.52
1:A:388:PRO:HD2	1:A:428:LYS:HG2	1.90	0.52
2:B:1546:LYS:HB3	2:B:1567:GLN:HG2	1.92	0.52
2:E:1631:TRP:CD2	2:E:1649:LEU:HD13	2.44	0.52
2:B:1314:GLU:OE1	2:B:1314:GLU:N	2.42	0.52
1:D:599:ASP:OD1	2:E:800:THR:HG21	2.08	0.52
2:E:977:GLU:OE2	2:E:979:ARG:NH2	2.42	0.52
3:F:943:CYS:HB3	3:F:990:LEU:HA	1.91	0.52
2:B:934:GLU:OE2	2:B:1353:LYS:HG2	2.10	0.52
3:C:987:LEU:N	3:C:991:VAL:O	2.40	0.52
1:A:242:PHE:HB3	1:A:379:PRO:HG2	1.91	0.52
1:A:199:VAL:O	2:B:937:ARG:NH1	2.43	0.52
2:E:1130:ILE:HD12	2:E:1133:LEU:HB2	1.92	0.52
1:A:459:SER:OG	1:A:474:ASN:HB2	2.10	0.51
1:D:32:ASN:HB2	1:D:643:GLY:C	2.31	0.51
2:B:916:VAL:HG23	2:B:919:HIS:HB2	1.92	0.51
2:E:1305:SER:HB3	3:F:1083:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HB2	1:A:535:TYR:CE2	2.43	0.51
1:A:595:LEU:HB2	2:B:774:ASN:HB2	1.91	0.51
2:B:754:ASP:H	3:C:980:ARG:NH1	2.09	0.51
3:C:1097:LEU:O	3:C:1101:GLY:HA2	2.10	0.51
1:D:29:ILE:HB	1:D:43:VAL:HB	1.91	0.51
1:D:653:GLN:HE22	2:E:1040:GLU:HG2	1.76	0.51
2:B:1495:PRO:HA	2:B:1496:GLU:HG2	1.92	0.51
1:D:97:LYS:HB3	1:D:98:SER:HB3	1.93	0.51
2:E:859:GLU:HB3	2:E:890:PRO:HD3	1.91	0.51
2:E:1076:THR:N	2:E:1120:GLU:OE1	2.43	0.51
2:B:911:GLU:HB2	2:B:926:ARG:HG3	1.93	0.50
2:B:1209:LYS:O	2:B:1213:THR:OG1	2.28	0.50
2:B:1387:GLU:HG3	2:B:1460:ALA:HB2	1.94	0.50
2:E:862:VAL:HG22	2:E:916:VAL:HG12	1.93	0.50
2:E:982:LEU:HB2	2:E:1320:ARG:HB2	1.93	0.50
2:E:1012:GLU:OE1	2:E:1126:HIS:ND1	2.24	0.50
2:E:1034:TRP:O	2:E:1038:GLY:N	2.43	0.50
2:E:1148:LEU:HD21	2:E:1199:MET:HE1	1.93	0.50
2:E:800:THR:HG22	2:E:801:THR:N	2.27	0.50
2:B:1547:THR:HG22	2:B:1565:ILE:HG12	1.94	0.49
1:A:583:LEU:N	2:B:791:MET:O	2.42	0.49
2:E:971:VAL:O	2:E:974:THR:OG1	2.22	0.49
2:B:756:ILE:HD12	2:B:922:SER:HB3	1.94	0.49
3:F:1018:ILE:HG22	3:F:1019:THR:HG23	1.94	0.49
1:D:329:THR:HG23	1:D:340:GLN:HG2	1.93	0.49
2:E:1136:ASN:OD1	2:E:1185:ARG:NH1	2.45	0.49
2:E:1209:LYS:O	2:E:1213:THR:OG1	2.31	0.49
1:D:493:LEU:HB2	1:D:532:VAL:HG22	1.95	0.49
2:E:800:THR:HG22	2:E:801:THR:H	1.78	0.49
2:E:1237:LEU:HD23	2:E:1278:ALA:HB1	1.94	0.49
3:F:953:LYS:HE3	3:F:974:ARG:HG3	1.94	0.49
2:E:1315:SER:HB2	2:E:1320:ARG:HH12	1.77	0.48
1:D:459:SER:OG	1:D:474:ASN:HB2	2.14	0.48
1:A:94:ARG:HG3	1:A:95:GLU:N	2.28	0.48
3:C:987:LEU:HD23	3:C:989:ASN:HB2	1.95	0.48
1:D:650:SER:HB2	1:D:652:GLN:OE1	2.14	0.48
1:A:101:GLY:HA3	1:A:102:ARG:HA	1.63	0.48
2:B:988:ALA:HA	2:B:1289:HIS:HA	1.94	0.48
1:D:109:GLN:HG3	1:D:118:GLU:HB3	1.95	0.48
1:D:397:VAL:HG12	1:D:409:LEU:HD22	1.96	0.48
1:D:508:ARG:NE	1:D:512:GLN:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLN:NE2	2:B:792:ASN:OD1	2.46	0.48
1:D:429:GLN:O	1:D:430:GLU:HG2	2.12	0.48
1:A:429:GLN:O	1:A:430:GLU:HG2	2.12	0.48
2:B:981:LEU:HB3	2:B:1319:LEU:HD11	1.95	0.48
1:D:372:LEU:HD21	1:D:422:ILE:HD13	1.95	0.48
2:E:874:SER:HB3	2:E:900:ILE:HG22	1.94	0.48
1:A:103:ASN:HB3	1:A:122:LEU:HD11	1.96	0.48
1:A:396:THR:O	1:A:397:VAL:HB	2.14	0.48
2:B:1237:LEU:HD23	2:B:1278:ALA:HB1	1.95	0.47
2:B:798:SER:HB3	2:B:802:TRP:HZ2	1.79	0.47
1:D:62:PHE:HA	1:D:63:PRO:HA	1.77	0.47
1:D:244:TYR:CE2	1:D:246:TYR:HB2	2.49	0.47
2:E:766:GLU:O	2:E:797:ASP:HB2	2.14	0.47
2:E:969:ASP:O	2:E:1351:LYS:N	2.44	0.47
2:E:1494:HIS:ND1	2:E:1495:PRO:HD2	2.30	0.47
1:D:334:SER:O	2:E:848:ARG:NH1	2.46	0.47
2:E:1314:GLU:OE1	2:E:1314:GLU:N	2.44	0.47
3:C:1064:ILE:HB	3:C:1087:TYR:HB2	1.96	0.47
1:D:69:LEU:HD13	1:D:88:PHE:HB2	1.97	0.47
1:D:566:LYS:HD2	1:D:584:LYS:HD2	1.95	0.47
1:A:35:ARG:HB2	1:A:38:SER:OG	2.15	0.47
2:B:1413:PRO:HA	2:B:1463:VAL:HG12	1.96	0.47
3:C:1046:ILE:HG12	3:C:1053:HIS:O	2.15	0.47
1:D:135:ASP:OD1	1:D:139:TYR:OH	2.17	0.47
1:A:35:ARG:HH22	1:A:498:GLY:HA3	1.79	0.47
1:A:329:THR:HG23	1:A:340:GLN:HG2	1.96	0.47
1:D:148:ARG:NH2	1:D:595:LEU:O	2.48	0.47
1:D:577:PRO:HD2	2:E:827:GLN:HG3	1.96	0.47
1:A:425:ARG:HG2	1:A:438:THR:HG22	1.96	0.46
1:A:132:ILE:HB	1:A:220:THR:OG1	2.15	0.46
1:D:35:ARG:HH22	1:D:498:GLY:HA3	1.80	0.46
1:D:85:ASN:OD1	1:D:85:ASN:N	2.47	0.46
3:F:954:LEU:HD23	3:F:970:LYS:O	2.14	0.46
2:B:1547:THR:HG22	2:B:1565:ILE:HA	1.98	0.46
1:D:580:GLN:NE2	3:F:1019:THR:O	2.38	0.46
2:E:1014:ASN:OD1	2:E:1055:GLN:NE2	2.45	0.46
1:A:205:LYS:HD2	1:A:207:ARG:CZ	2.45	0.46
1:A:394:GLU:HG2	1:A:396:THR:C	2.36	0.46
2:B:841:ARG:NH1	2:B:1509:GLU:HB3	2.28	0.46
2:B:978:THR:HB	2:B:1324:THR:HG23	1.98	0.46
2:B:1138:GLU:OE2	2:B:1141:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLU:HG3	1:D:88:PHE:HB3	1.96	0.46
2:E:1136:ASN:C	2:E:1138:GLU:H	2.17	0.46
1:A:45:GLU:HG2	1:A:83:MET:HG3	1.97	0.46
2:B:971:VAL:O	2:B:974:THR:OG1	2.21	0.46
1:A:628:THR:OG1	1:A:641:ASP:HB3	2.16	0.46
2:B:1532:ARG:NH2	2:B:1629:GLU:OE2	2.49	0.46
1:D:365:LYS:HD2	1:D:455:TYR:HB3	1.98	0.46
1:D:130:LEU:HB2	1:D:218:PHE:CD1	2.50	0.46
2:E:799:ILE:HG23	2:E:826:MET:HA	1.97	0.46
3:F:978:TYR:HD2	3:F:1002:LYS:HG2	1.80	0.46
3:F:1094:ARG:HG2	3:F:1095:CYS:H	1.79	0.46
1:A:360:THR:O	1:A:362:LYS:NZ	2.43	0.46
3:F:1127:GLY:HA2	3:F:1128:PRO:HD3	1.80	0.46
2:E:844:GLN:HA	2:E:901:VAL:HG22	1.97	0.45
1:A:129:TYR:CE2	1:A:154:HIS:HA	2.51	0.45
1:D:101:GLY:HA3	1:D:102:ARG:HA	1.60	0.45
1:D:591:ALA:HB2	2:E:810:SER:HB2	1.98	0.45
2:E:1554:LEU:HD21	2:E:1591:ARG:HD2	1.98	0.45
1:D:311:VAL:HG12	1:D:313:ASN:H	1.81	0.45
2:E:1077:TRP:CZ2	2:E:1130:ILE:HA	2.51	0.45
2:B:1438:PHE:HE1	2:B:1466:TYR:HB3	1.81	0.45
1:D:281:ARG:NH2	1:D:342:GLU:OE2	2.47	0.45
1:D:347:PRO:HG2	1:D:379:PRO:HB2	1.97	0.45
2:E:1359:ASN:HB2	2:E:1360:LYS:HD2	1.98	0.45
1:A:32:ASN:HB2	1:A:643:GLY:C	2.37	0.45
3:F:1064:ILE:HB	3:F:1087:TYR:HB2	1.98	0.45
3:F:1106:GLU:H	3:F:1134:ILE:N	2.14	0.45
2:B:868:HIS:ND1	2:B:876:ALA:O	2.48	0.45
2:B:1584:PHE:HA	2:B:1620:TYR:O	2.16	0.45
1:D:460:VAL:HG13	1:D:471:LEU:HD11	1.98	0.45
2:E:941:THR:HA	2:E:1345:VAL:HG22	1.98	0.45
2:B:1029:ASP:HA	2:B:1034:TRP:HE1	1.81	0.45
1:A:351:SER:HA	1:A:352:PRO:HD3	1.86	0.45
3:C:1007:PRO:HB2	3:C:1015:VAL:HG11	1.99	0.45
2:E:798:SER:HB2	2:E:802:TRP:HZ2	1.82	0.45
1:A:496:ASN:OD1	1:A:497:LYS:HE3	2.17	0.44
2:B:1565:ILE:HD12	2:B:1576:VAL:HG21	1.98	0.44
2:E:1106:TRP:CD1	2:E:1110:GLU:HG3	2.53	0.44
1:D:44:LEU:HD13	1:D:55:VAL:HG11	1.99	0.44
1:D:465:LEU:HD22	1:D:555:VAL:HG22	1.98	0.44
1:A:68:VAL:HG11	1:A:90:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:945:ALA:HA	3:C:946:PRO:HD3	1.84	0.44
1:D:52:ASP:OD1	1:D:78:PRO:HD2	2.17	0.44
2:E:841:ARG:NH1	2:E:1509:GLU:O	2.50	0.44
1:A:474:ASN:HB3	1:A:514:LEU:HD11	1.98	0.44
1:A:577:PRO:HD2	2:B:827:GLN:HG3	2.00	0.44
2:B:958:GLN:NE2	2:B:960:GLU:OE2	2.44	0.44
2:B:1174:ASP:OD1	2:B:1201:ARG:NH2	2.30	0.44
1:A:130:LEU:HB2	1:A:218:PHE:CD1	2.52	0.44
1:A:281:ARG:NH2	1:A:342:GLU:OE2	2.44	0.44
2:E:916:VAL:HG23	2:E:919:HIS:HB2	1.99	0.44
2:E:1523:SER:HB2	2:E:1526:LYS:HA	1.98	0.44
2:E:962:ILE:HD11	2:E:1342:LEU:HD21	1.99	0.44
2:B:1036:LYS:HB2	2:B:1036:LYS:HE2	1.82	0.44
2:B:1214:ALA:HA	2:B:1219:ARG:O	2.18	0.44
1:D:658:ALA:HB1	2:E:1035:GLU:OE2	2.17	0.44
3:F:946:PRO:HD3	3:F:963:PHE:HE2	1.82	0.44
1:A:245:ILE:HD11	1:A:320:VAL:HG22	2.00	0.43
1:A:493:LEU:HB2	1:A:532:VAL:HG22	2.00	0.43
2:B:1185:ARG:O	2:B:1189:VAL:HG23	2.17	0.43
2:B:1152:GLN:NE2	2:B:1198:GLN:OE1	2.51	0.43
2:B:1325:LYS:HE2	2:B:1325:LYS:HB3	1.82	0.43
1:D:392:GLN:HA	1:D:393:GLY:HA2	1.59	0.43
2:B:1200:GLY:O	2:B:1203:LYS:NZ	2.47	0.43
1:D:57:VAL:HG21	1:D:86:VAL:HG21	1.99	0.43
1:A:544:ARG:HB3	1:A:652:GLN:NE2	2.33	0.43
1:D:133:GLN:HB2	1:D:611:LEU:HD22	1.99	0.43
2:B:781:PRO:HA	2:B:782:PRO:HD3	1.81	0.43
3:C:1094:ARG:HG2	3:C:1095:CYS:H	1.83	0.43
1:D:628:THR:OG1	1:D:641:ASP:HB3	2.18	0.43
2:E:1604:MET:HA	2:E:1627:TRP:O	2.19	0.43
2:B:1293:ASN:OD1	2:B:1312:HIS:ND1	2.44	0.43
2:E:1536:ALA:O	2:E:1570:LYS:NZ	2.51	0.43
1:D:69:LEU:HD21	1:D:72:GLU:HG2	1.99	0.43
1:D:580:GLN:NE2	3:F:1020:ASP:HA	2.34	0.43
2:E:1255:TRP:O	2:E:1259:GLN:HG2	2.18	0.43
1:A:35:ARG:NH2	1:A:498:GLY:HA3	2.34	0.43
1:A:62:PHE:HA	1:A:63:PRO:HA	1.75	0.43
1:A:229:LEU:HA	1:A:230:PRO:HD3	1.87	0.43
1:A:244:TYR:CE2	1:A:246:TYR:HB2	2.54	0.43
1:D:32:ASN:HA	1:D:645:THR:HG23	2.00	0.43
1:D:455:TYR:HD2	1:D:478:ARG:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:969:ASP:O	2:E:1351:LYS:HB2	2.18	0.43
2:E:1533:LEU:HD23	2:E:1533:LEU:HA	1.86	0.43
1:A:372:LEU:HD21	1:A:422:ILE:HD13	2.00	0.43
2:B:969:ASP:O	2:B:1351:LYS:HB2	2.19	0.43
2:B:1368:LYS:HA	2:B:1369:PRO:HD3	1.94	0.43
3:C:943:CYS:N	3:C:990:LEU:HD22	2.34	0.43
1:D:473:VAL:HG11	1:D:531:LEU:HD21	2.01	0.43
1:D:475:PHE:O	1:D:514:LEU:HA	2.19	0.43
1:A:58:THR:HG22	1:A:70:SER:O	2.19	0.42
3:C:1058:PRO:HA	3:C:1059:PRO:HD3	1.68	0.42
2:E:1363:LEU:HD21	2:E:1477:VAL:HG12	2.01	0.42
2:E:1494:HIS:HB3	2:E:1497:LYS:HB2	2.00	0.42
2:E:1661:CYS:HA	2:E:1662:PRO:HD3	1.92	0.42
1:A:274:GLY:HA3	1:A:325:TYR:CZ	2.54	0.42
1:D:130:LEU:HD23	1:D:151:THR:HA	2.00	0.42
2:B:1106:TRP:CD1	2:B:1110:GLU:HG3	2.54	0.42
2:B:1309:HIS:CG	2:B:1320:ARG:HG2	2.55	0.42
2:E:1073:ALA:HA	2:E:1074:PRO:HD3	1.91	0.42
2:E:1409:THR:HG22	2:E:1473:GLN:H	1.82	0.42
1:A:269:ALA:HB2	1:A:330:VAL:HG22	2.00	0.42
1:A:277:ASP:HA	1:A:278:GLY:HA2	1.69	0.42
2:B:1194:TYR:CE1	2:B:1238:LEU:HB3	2.54	0.42
1:D:352:PRO:O	1:D:379:PRO:HD3	2.19	0.42
1:D:448:THR:OG1	1:D:449:VAL:N	2.51	0.42
1:A:32:ASN:HD22	1:A:32:ASN:HA	1.69	0.42
1:A:169:ASN:OD1	1:A:173:ILE:N	2.53	0.42
2:E:1261:TYR:CZ	2:E:1263:GLY:HA2	2.54	0.42
1:D:238:PRO:HB2	1:D:240:GLU:O	2.19	0.42
1:D:274:GLY:HA3	1:D:325:TYR:CZ	2.54	0.42
2:E:798:SER:HB2	2:E:802:TRP:CZ2	2.55	0.42
2:E:1504:LYS:O	2:E:1558:PHE:HZ	2.02	0.42
2:E:1042:ARG:NH1	2:E:1046:LEU:HD11	2.34	0.42
3:F:1106:GLU:N	3:F:1134:ILE:N	2.67	0.42
2:B:1519:PHE:HD1	2:B:1521:GLN:H	1.67	0.42
1:A:69:LEU:HD13	1:A:88:PHE:HB2	2.01	0.42
1:A:536:THR:OG1	1:A:544:ARG:HD2	2.19	0.42
3:C:1018:ILE:HG22	3:C:1019:THR:HG23	2.02	0.42
3:F:1003:SER:HB2	3:F:1021:ILE:HG13	2.01	0.42
1:A:46:ALA:HB3	1:A:82:HIS:HB3	2.01	0.42
1:A:603:PHE:O	1:A:607:LYS:HG3	2.19	0.42
2:B:1317:SER:N	2:B:1318:LEU:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1591:ARG:HG2	2:B:1592:GLU:N	2.35	0.42
2:E:958:GLN:NE2	2:E:960:GLU:OE2	2.41	0.42
2:E:962:ILE:HD13	2:E:1344:VAL:HG21	2.01	0.42
3:F:1007:PRO:HA	3:F:1008:PRO:HD3	1.82	0.42
2:B:895:SER:O	2:B:1442:ASN:ND2	2.53	0.41
2:E:1387:GLU:HG3	2:E:1460:ALA:HB2	2.02	0.41
3:F:1023:VAL:HA	3:F:1045:CYS:SG	2.60	0.41
3:F:1064:ILE:HA	3:F:1065:PRO:HD3	1.96	0.41
1:A:271:VAL:HG11	1:A:300:VAL:HG11	2.02	0.41
1:A:392:GLN:HA	1:A:393:GLY:C	2.40	0.41
2:B:758:GLU:HG2	2:B:913:LYS:HD2	2.02	0.41
2:B:932:VAL:HG12	2:B:933:PRO:O	2.20	0.41
1:A:390:ALA:HB3	1:A:427:LYS:HE2	2.03	0.41
2:B:1042:ARG:NH1	2:B:1046:LEU:HD11	2.35	0.41
2:E:978:THR:HB	2:E:1324:THR:HG23	2.02	0.41
2:E:1152:GLN:OE1	2:E:1198:GLN:NE2	2.50	0.41
1:A:68:VAL:HG12	1:A:91:PRO:HD2	2.02	0.41
2:E:826:MET:HG2	2:E:827:GLN:N	2.36	0.41
3:C:1069:PRO:HA	3:C:1070:PRO:HD3	1.95	0.41
1:A:130:LEU:HD23	1:A:151:THR:HA	2.03	0.41
1:D:112:PHE:C	1:D:114:THR:H	2.22	0.41
1:D:433:GLU:HA	1:D:436:GLN:HG2	2.01	0.41
1:A:481:ARG:HH22	1:D:480:ASP:HB2	1.85	0.41
1:D:530:ARG:NH1	1:D:624:ASP:OD2	2.51	0.41
2:E:1053:TYR:CZ	2:E:1057:LEU:HD11	2.55	0.41
2:E:1204:GLY:HA3	2:E:1205:PRO:HD3	1.87	0.41
1:A:44:LEU:HD13	1:A:55:VAL:HG11	2.02	0.41
1:A:276:GLN:HB3	1:A:323:SER:OG	2.21	0.41
1:A:388:PRO:HA	1:A:399:SER:O	2.21	0.41
2:B:982:LEU:HD23	2:B:1342:LEU:HD13	2.03	0.41
2:B:1494:HIS:HA	2:B:1495:PRO:HD3	1.71	0.41
1:D:32:ASN:HA	1:D:32:ASN:HD22	1.62	0.41
1:D:67:LEU:HD11	1:D:70:SER:HB3	2.02	0.41
2:E:1065:ALA:HB2	2:E:1106:TRP:CD2	2.56	0.41
2:E:1265:GLY:N	2:E:1268:SER:OG	2.54	0.41
2:E:1370:ALA:HB2	2:E:1385:ILE:HG13	2.02	0.41
1:A:324:LEU:HB2	1:A:346:ILE:HB	2.02	0.41
2:E:865:GLU:OE2	2:E:881:ARG:NH1	2.53	0.41
2:E:1148:LEU:HD21	2:E:1199:MET:CE	2.51	0.41
2:E:1155:LYS:O	2:E:1159:GLU:N	2.53	0.41
2:B:754:ASP:OD2	2:B:918:HIS:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1248:PHE:O	2:B:1251:PRO:HD2	2.21	0.40
2:B:1528:THR:OG1	2:B:1531:GLU:HG2	2.21	0.40
2:E:781:PRO:HA	2:E:782:PRO:HD3	1.90	0.40
2:E:1188:THR:HA	2:E:1191:ILE:HG22	2.03	0.40
2:B:1586:SER:HA	2:B:1587:PRO:HD3	1.95	0.40
1:D:355:ILE:HG23	1:D:374:VAL:HG13	2.02	0.40
1:D:488:ARG:HD2	1:D:488:ARG:HA	1.86	0.40
2:E:801:THR:HG22	2:E:824:THR:HA	2.04	0.40
2:E:1547:THR:HG22	2:E:1565:ILE:HG12	2.02	0.40
1:A:93:ASN:O	1:A:94:ARG:HG2	2.21	0.40
2:B:789:LYS:HE2	2:B:789:LYS:HB2	1.96	0.40
2:B:826:MET:HG2	2:B:827:GLN:N	2.36	0.40
1:D:78:PRO:C	1:D:80:THR:H	2.24	0.40
2:E:1245:ASP:O	2:E:1249:VAL:HG23	2.21	0.40
2:E:1325:LYS:HE2	2:E:1325:LYS:HB3	1.84	0.40
2:E:1368:LYS:HA	2:E:1369:PRO:HD3	1.93	0.40
2:E:1588:ILE:O	2:E:1589:LYS:CG	2.70	0.40
1:A:506:GLN:NE2	1:A:507:VAL:O	2.52	0.40
2:B:977:GLU:OE2	2:B:979:ARG:NH2	2.54	0.40
2:B:1255:TRP:O	2:B:1259:GLN:HG2	2.21	0.40
2:E:1012:GLU:OE2	2:E:1125:ILE:HG13	2.22	0.40
2:E:1060:ARG:HD2	2:E:1099:VAL:HG13	2.04	0.40
2:E:1297:SER:OG	2:E:1333:THR:HB	2.21	0.40
1:A:352:PRO:O	1:A:379:PRO:HD3	2.21	0.40
1:D:45:GLU:OE1	1:D:534:TYR:OH	2.26	0.40
1:D:90:ILE:HA	1:D:91:PRO:HD3	1.90	0.40
2:E:1248:PHE:O	2:E:1251:PRO:HD2	2.21	0.40
3:F:946:PRO:HD3	3:F:963:PHE:CE2	2.56	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	640/645 (99%)	624 (98%)	14 (2%)	2 (0%)	41 71
1	D	640/645 (99%)	625 (98%)	15 (2%)	0	100 100
2	B	899/915 (98%)	866 (96%)	33 (4%)	0	100 100
2	E	899/915 (98%)	868 (97%)	31 (3%)	0	100 100
3	C	192/196 (98%)	175 (91%)	17 (9%)	0	100 100
3	F	192/196 (98%)	179 (93%)	13 (7%)	0	100 100
All	All	3462/3512 (99%)	3337 (96%)	123 (4%)	2 (0%)	51 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	THR
1	A	397	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	566/567 (100%)	561 (99%)	5 (1%)	78 87
1	D	566/567 (100%)	560 (99%)	6 (1%)	73 85
2	B	798/810 (98%)	794 (100%)	4 (0%)	88 93
2	E	798/810 (98%)	791 (99%)	7 (1%)	78 87
3	C	167/173 (96%)	163 (98%)	4 (2%)	49 73
3	F	167/173 (96%)	164 (98%)	3 (2%)	59 78
All	All	3062/3100 (99%)	3033 (99%)	29 (1%)	78 87

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	93	ASN
1	A	95	GLU

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Mol	Chain	Res	Type
1	A	391	VAL
1	A	395	ASP
2	B	1293	ASN
2	B	1453	HIS
2	B	1605	TRP
2	B	1637	CYS
3	C	986	CYS
3	C	998	VAL
3	C	1004	CYS
3	C	1031	CYS
1	D	32	ASN
1	D	85	ASN
1	D	265	VAL
1	D	391	VAL
1	D	607	LYS
1	D	656	GLN
2	E	934	GLU
2	E	1293	ASN
2	E	1357	THR
2	E	1450	LYS
2	E	1518	CYS
2	E	1605	TRP
2	E	1637	CYS
3	F	986	CYS
3	F	997	ASP
3	F	1031	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	580	GLN
1	D	32	ASN
1	D	653	GLN
3	F	1012	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)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	NAG	A	1063	1	14,14,15	0.51	0	17,19,21	1.98	2 (11%)
4	NAG	D	1063	1	14,14,15	0.50	0	17,19,21	0.73	0

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
4	NAG	A	1063	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	1063	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1063	NAG	C1-O5-C5	5.61	119.79	112.19
4	A	1063	NAG	O5-C1-C2	4.97	119.13	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1063	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1063	NAG	1	0

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	642/645 (99%)	0.32	19 (2%) 50 49	75, 118, 176, 230	0
1	D	642/645 (99%)	0.33	24 (3%) 41 38	69, 115, 172, 243	0
2	B	903/915 (98%)	0.79	117 (12%) 3 3	72, 154, 220, 261	0
2	E	903/915 (98%)	0.48	73 (8%) 12 11	65, 134, 196, 234	0
3	C	194/196 (98%)	1.09	45 (23%) 0 1	96, 162, 278, 346	0
3	F	194/196 (98%)	1.56	55 (28%) 0 0	111, 201, 248, 316	0
All	All	3478/3512 (99%)	0.60	333 (9%) 8 8	65, 135, 218, 346	0

All (333) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1107	LEU	11.0
1	D	98	SER	9.8
3	F	1109	GLY	8.7
3	C	961	SER	7.6
3	C	981	PRO	7.2
2	B	1155	LYS	6.5
1	D	96	PHE	6.4
2	B	1525	ASP	6.4
2	B	1556	ASN	6.4
2	B	1205	PRO	6.4
2	B	1371	PRO	6.3
3	F	1134	ILE	6.3
1	D	97	LYS	5.9
2	E	947	LEU	5.8
2	B	1557	ASP	5.8
2	E	968	SER	5.8
3	F	1075	GLY	5.7
2	B	1067	ALA	5.6
2	B	1162	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	1090	VAL	5.5
1	D	95	GLU	5.4
3	F	974	ARG	5.4
2	B	1212	THR	5.4
2	B	861	LYS	5.2
3	C	948	HIS	5.1
1	D	403	GLY	5.0
2	B	1065	ALA	5.0
2	E	1307	ILE	4.9
2	B	1394	GLY	4.9
3	C	990	LEU	4.9
2	B	1599	LYS	4.8
3	C	960	ALA	4.8
3	C	956	THR	4.7
2	B	1119	GLN	4.5
2	E	801	THR	4.5
3	C	955	LYS	4.5
3	C	958	THR	4.5
3	F	971	TYR	4.5
2	B	860	LEU	4.4
2	B	1580	GLN	4.4
1	A	79	ALA	4.4
3	C	941	GLY	4.4
2	E	941	THR	4.3
2	B	1161	GLN	4.3
2	E	1317	SER	4.3
2	E	959	LYS	4.3
2	B	1163	ASN	4.3
1	D	71	SER	4.3
2	B	1137	ASN	4.3
3	C	957	GLN	4.2
2	E	1304	SER	4.2
3	C	944	GLN	4.2
3	F	981	PRO	4.2
2	E	961	ASP	4.2
1	A	95	GLU	4.2
2	B	760	ASN	4.2
2	B	1583	THR	4.1
2	B	1083	VAL	4.1
3	F	1098	GLY	4.0
3	C	980	ARG	4.0
3	C	986	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	1460	ALA	4.0
3	C	970	LYS	4.0
3	F	948	HIS	4.0
2	B	1071	LYS	3.9
2	E	1461	PHE	3.9
1	D	100	LYS	3.9
3	C	942	HIS	3.9
3	F	956	THR	3.9
1	A	98	SER	3.8
3	C	993	SER	3.8
2	B	1537	CYS	3.8
2	B	1609	SER	3.8
3	C	959	ASN	3.8
3	C	954	LEU	3.7
3	C	968	SER	3.7
3	F	1106	GLU	3.7
2	B	920	PHE	3.7
1	A	319	LEU	3.7
2	B	1563	MET	3.7
2	B	1608	SER	3.6
3	F	945	ALA	3.6
3	C	946	PRO	3.6
1	D	429	GLN	3.6
3	C	987	LEU	3.6
3	C	994	SER	3.6
3	F	970	LYS	3.6
3	C	985	THR	3.6
3	C	989	ASN	3.6
1	D	52	ASP	3.6
3	F	1103	LYS	3.5
2	B	1218	ASN	3.5
3	F	969	LEU	3.5
3	F	992	TRP	3.5
2	B	1121	ASP	3.5
2	E	1347	MET	3.5
2	B	1104	VAL	3.5
1	A	313	ASN	3.5
2	B	1125	ILE	3.5
3	C	982	PHE	3.5
2	E	753	GLU	3.4
3	F	961	SER	3.4
3	C	945	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	1074	PRO	3.4
2	B	1156	ASP	3.4
2	B	1306	LYS	3.4
1	D	396	THR	3.4
3	C	983	SER	3.4
2	B	1619	SER	3.4
3	C	943	CYS	3.3
2	E	1537	CYS	3.3
2	E	1162	VAL	3.3
2	B	1560	GLU	3.3
2	E	1316	ALA	3.3
2	E	1305	SER	3.3
2	B	1151	LEU	3.3
3	C	1096	ASN	3.3
1	A	97	LYS	3.3
3	F	986	CYS	3.3
3	F	1018	ILE	3.3
3	F	953	LYS	3.3
1	D	99	GLU	3.2
2	B	1575	GLU	3.2
2	B	1615	LYS	3.2
2	E	1409	THR	3.2
2	B	1117	VAL	3.2
2	B	923	ASP	3.2
2	E	752	ASP	3.2
3	F	979	GLY	3.2
3	F	1119	ASP	3.2
2	B	1259	GLN	3.2
3	C	949	PHE	3.1
2	B	1620	TYR	3.1
3	C	969	LEU	3.1
2	B	1073	ALA	3.1
2	E	943	ALA	3.1
2	B	1413	PRO	3.1
2	B	1618	LEU	3.1
2	B	1438	PHE	3.1
2	E	918	HIS	3.1
3	C	991	VAL	3.1
3	C	953	LYS	3.0
1	D	392	GLN	3.0
2	E	1598	GLU	3.0
3	F	952	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	987	LEU	3.0
2	B	1369	PRO	3.0
2	B	1220	TRP	3.0
2	B	1182	ASN	3.0
2	B	1558	PHE	3.0
2	B	917	TYR	3.0
3	F	1074	ASN	3.0
3	F	1118	ASN	3.0
3	C	971	TYR	3.0
2	B	1461	PHE	3.0
3	F	943	CYS	3.0
2	E	1354	ASP	2.9
2	E	1311	ILE	2.9
3	F	1019	THR	2.9
2	B	1120	GLU	2.9
2	B	1542	ASP	2.9
3	F	941	GLY	2.9
3	F	994	SER	2.9
2	E	1333	THR	2.9
2	E	1524	ASP	2.9
1	D	397	VAL	2.9
2	B	1066	PHE	2.9
2	E	1370	ALA	2.9
2	E	1327	ASN	2.9
2	E	1663	ASN	2.9
1	D	67	LEU	2.9
3	C	995	PRO	2.9
2	B	1562	ILE	2.9
3	C	962	ASP	2.9
2	B	1062	PRO	2.9
3	F	978	TYR	2.8
2	E	1351	LYS	2.8
2	E	1315	SER	2.8
3	C	1103	LYS	2.8
3	F	980	ARG	2.8
2	B	1034	TRP	2.7
2	E	1393	ARG	2.7
1	D	404	ASP	2.7
2	E	1348	TYR	2.7
2	B	1138	GLU	2.7
3	F	996	LYS	2.7
1	D	574	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	946	PRO	2.7
2	B	1606	GLY	2.7
2	B	1663	ASN	2.7
3	F	959	ASN	2.7
2	B	1402	ILE	2.7
2	B	1164	SER	2.7
3	F	1012	ASN	2.7
1	A	573	ARG	2.7
2	E	945	ARG	2.6
3	F	964	PRO	2.6
1	A	337	ASP	2.6
2	B	1210	PHE	2.6
1	D	94	ARG	2.6
2	B	1635	ASP	2.6
2	E	1525	ASP	2.6
2	B	1584	PHE	2.6
2	B	1305	SER	2.6
2	B	1579	GLY	2.6
2	E	1622	ILE	2.6
2	E	1556	ASN	2.5
2	B	1543	TYR	2.5
2	E	946	THR	2.5
1	A	253	VAL	2.5
2	B	1095	ILE	2.5
3	F	1133	ILE	2.5
2	B	1384	MET	2.5
2	E	1616	PRO	2.5
3	F	957	GLN	2.5
2	E	1548	ARG	2.5
1	A	99	GLU	2.5
1	D	269	ALA	2.5
2	E	1606	GLY	2.5
2	B	1565	ILE	2.5
2	E	1068	ALA	2.5
2	B	1248	PHE	2.5
2	E	923	ASP	2.5
3	C	963	PHE	2.5
2	B	1622	ILE	2.5
2	B	1638	GLN	2.5
1	A	572	ASP	2.4
1	A	96	PHE	2.4
2	B	1632	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	1370	ALA	2.4
3	F	1083	GLU	2.4
2	E	1332	VAL	2.4
3	F	955	LYS	2.4
1	A	384	ALA	2.4
1	A	383	PRO	2.4
2	B	996	ASP	2.4
2	E	1528	THR	2.4
2	E	980	ILE	2.4
2	E	1355	GLN	2.4
2	B	995	VAL	2.3
3	C	974	ARG	2.3
1	D	543	GLN	2.3
2	E	967	LEU	2.3
2	E	1386	LEU	2.3
3	F	1128	PRO	2.3
2	B	934	GLU	2.3
2	B	1645	GLN	2.3
3	F	1080	THR	2.3
2	B	916	VAL	2.3
2	B	1616	PRO	2.3
2	E	781	PRO	2.3
3	F	1082	ARG	2.3
2	B	1033	GLN	2.3
2	B	1392	TYR	2.3
3	F	1120	ASP	2.3
2	E	1438	PHE	2.3
2	E	1322	GLU	2.3
2	E	1342	LEU	2.3
2	B	1571	SER	2.3
3	F	1110	GLU	2.3
2	E	1549	LEU	2.3
2	B	1146	PHE	2.3
2	B	1383	THR	2.3
2	B	1446	ILE	2.3
2	B	1365	VAL	2.3
2	B	982	LEU	2.3
2	E	1137	ASN	2.2
2	E	1319	LEU	2.2
2	B	1124	VAL	2.2
2	B	800	THR	2.2
2	B	1181	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	312	GLN	2.2
2	B	1069	PHE	2.2
2	E	957	VAL	2.2
2	B	1595	LYS	2.2
3	F	976	GLU	2.2
1	D	383	PRO	2.2
1	A	231	SER	2.2
2	E	1334	ALA	2.2
2	E	1413	PRO	2.2
2	B	1307	ILE	2.2
2	B	922	SER	2.2
2	E	1009	GLY	2.2
3	C	1104	VAL	2.2
3	F	1099	SER	2.2
3	F	1077	PHE	2.2
3	F	988	ASP	2.2
1	D	568	GLY	2.2
2	B	1528	THR	2.2
3	C	992	TRP	2.1
2	E	1361	PHE	2.1
2	B	1600	LYS	2.1
2	E	755	ILE	2.1
3	C	973	CYS	2.1
2	B	1227	LEU	2.1
2	E	1402	ILE	2.1
2	B	1213	THR	2.1
2	E	1562	ILE	2.1
3	F	1078	ILE	2.1
3	F	1004	CYS	2.1
2	B	1184	GLN	2.1
2	E	954	ARG	2.1
3	C	978	TYR	2.1
2	B	942	VAL	2.1
2	B	1038	GLY	2.1
2	B	1547	THR	2.1
2	E	1330	PHE	2.1
2	B	1439	SER	2.1
2	E	940	LYS	2.1
3	F	954	LEU	2.1
2	B	752	ASP	2.1
2	E	1615	LYS	2.1
2	B	1482	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	1133	ILE	2.1
2	B	884	GLN	2.0
2	B	1611	PHE	2.0
1	D	386	ARG	2.0
2	E	861	LYS	2.0
2	E	964	PRO	2.0
1	A	398	GLN	2.0
1	A	397	VAL	2.0
2	B	1585	ILE	2.0
3	C	966	GLY	2.0
3	F	1069	PRO	2.0
2	E	1555	SER	2.0
2	B	1544	VAL	2.0
2	E	924	GLY	2.0
1	D	76	LEU	2.0
2	E	1554	LEU	2.0
2	E	1218	ASN	2.0
3	F	1061	CYS	2.0
1	D	70	SER	2.0
1	A	590	GLY	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
4	NAG	A	1063	14/15	0.82	0.28	106,127,145,146	0
4	NAG	D	1063	14/15	0.88	0.26	87,134,158,164	0

6.5 Other polymers (i)

There are no such residues in this entry.