



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:53 PM UTC

PDB ID : 5FO9 / pdb_00005fo9
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

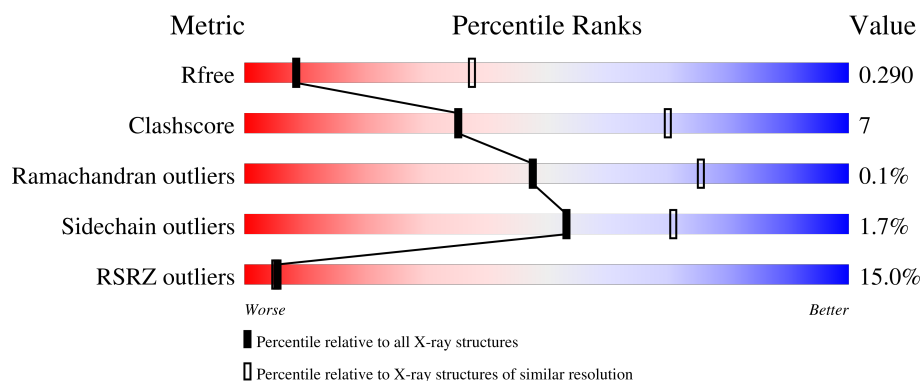
1 Overall quality at a glance

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	10% 76% 22% .
1	D	645	10% 79% 20% .
2	B	915	19% 82% 17% .
2	E	915	13% 79% 19% .
3	C	196	24% 76% 22% ..

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Mol	Chain	Length	Quality of chain
3	F	196	

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

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			

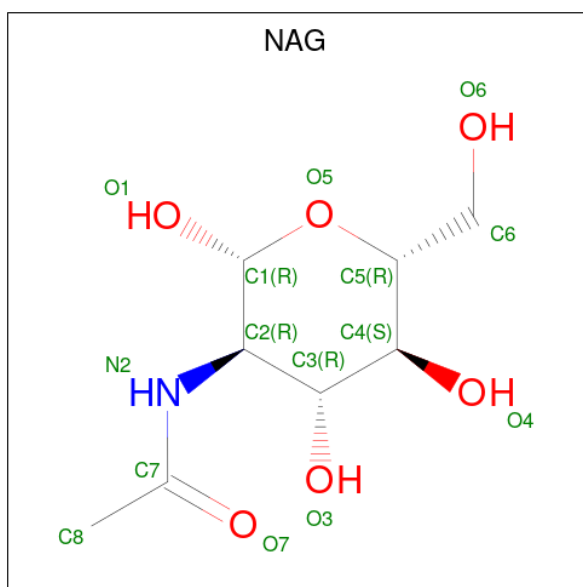
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).

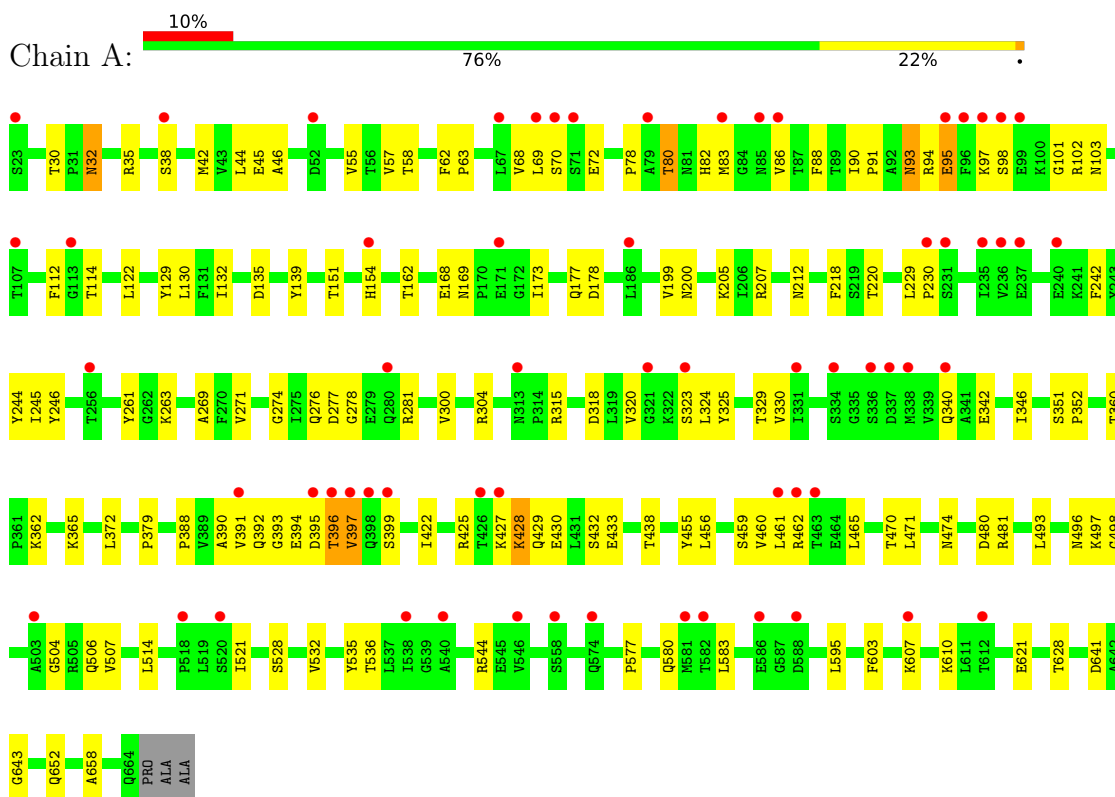


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

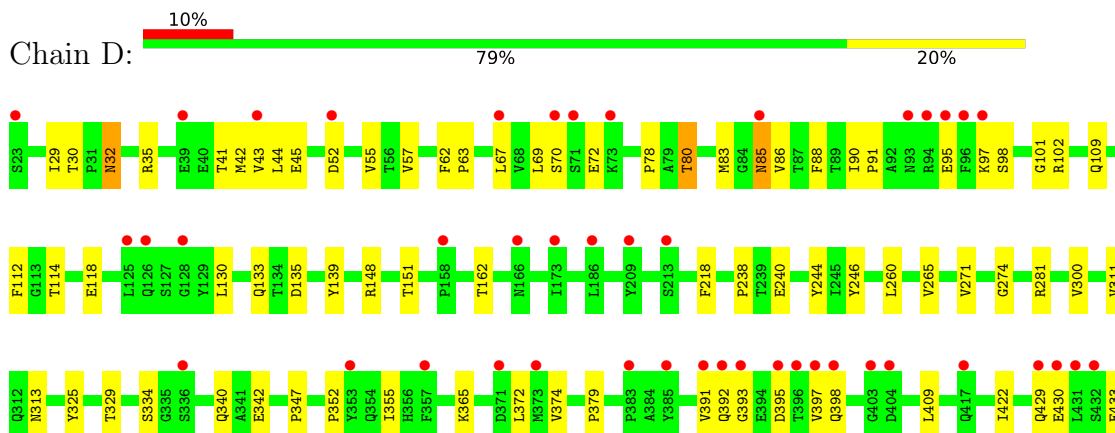
3 Residue-property plots

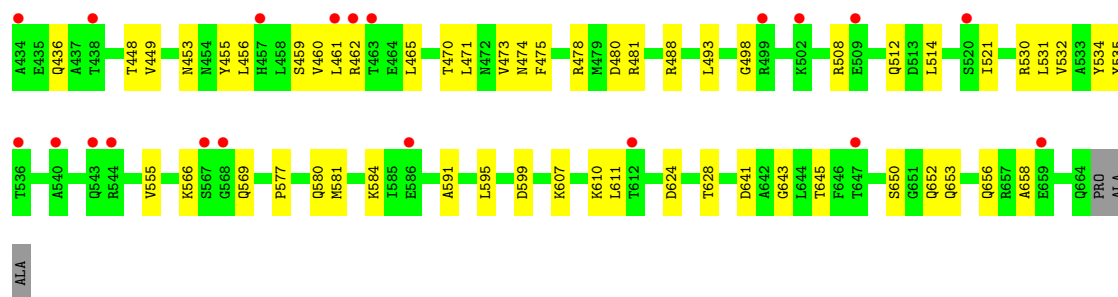
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

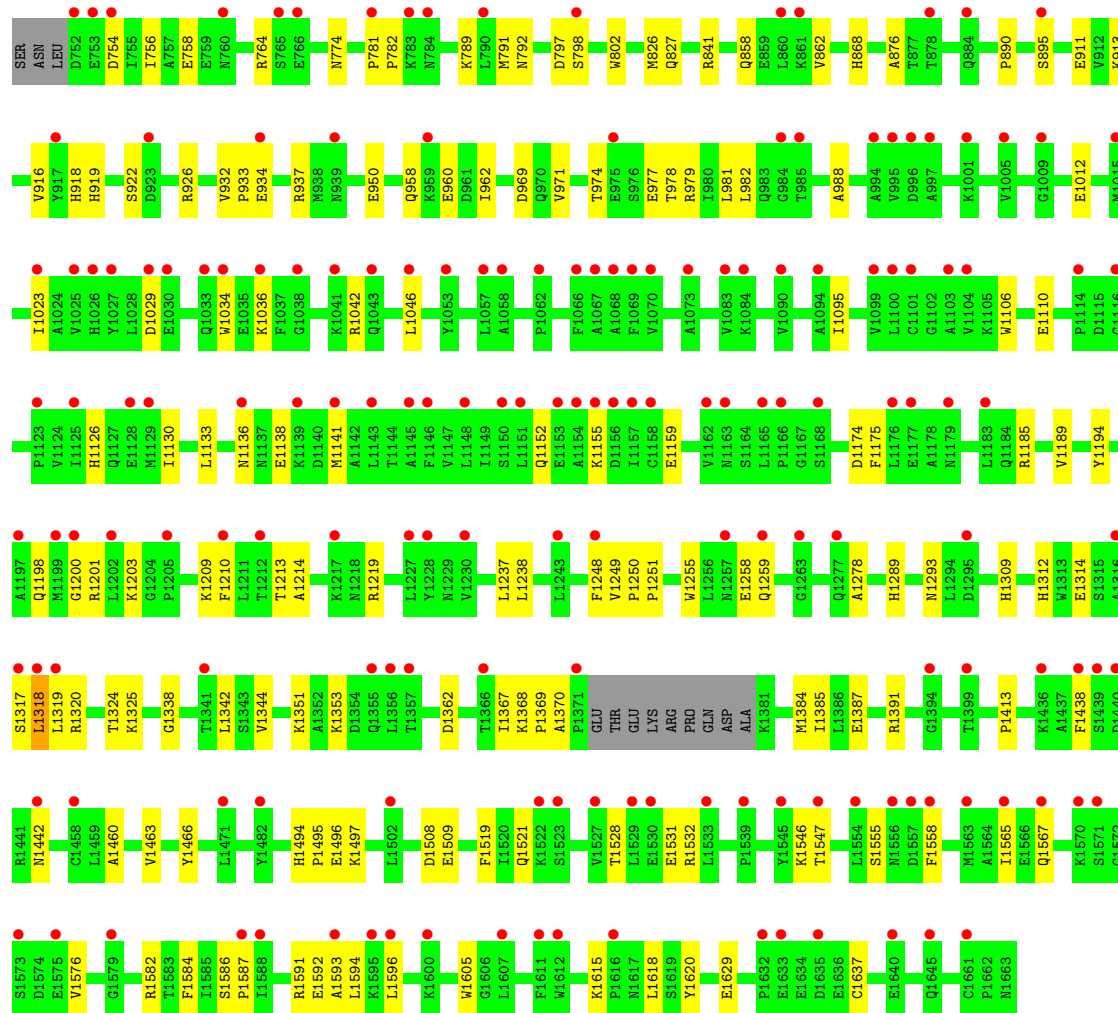


• Molecule 1: COMPLEMENT C3 BETA CHAIN

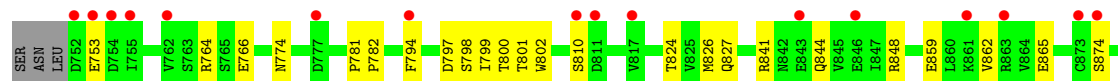


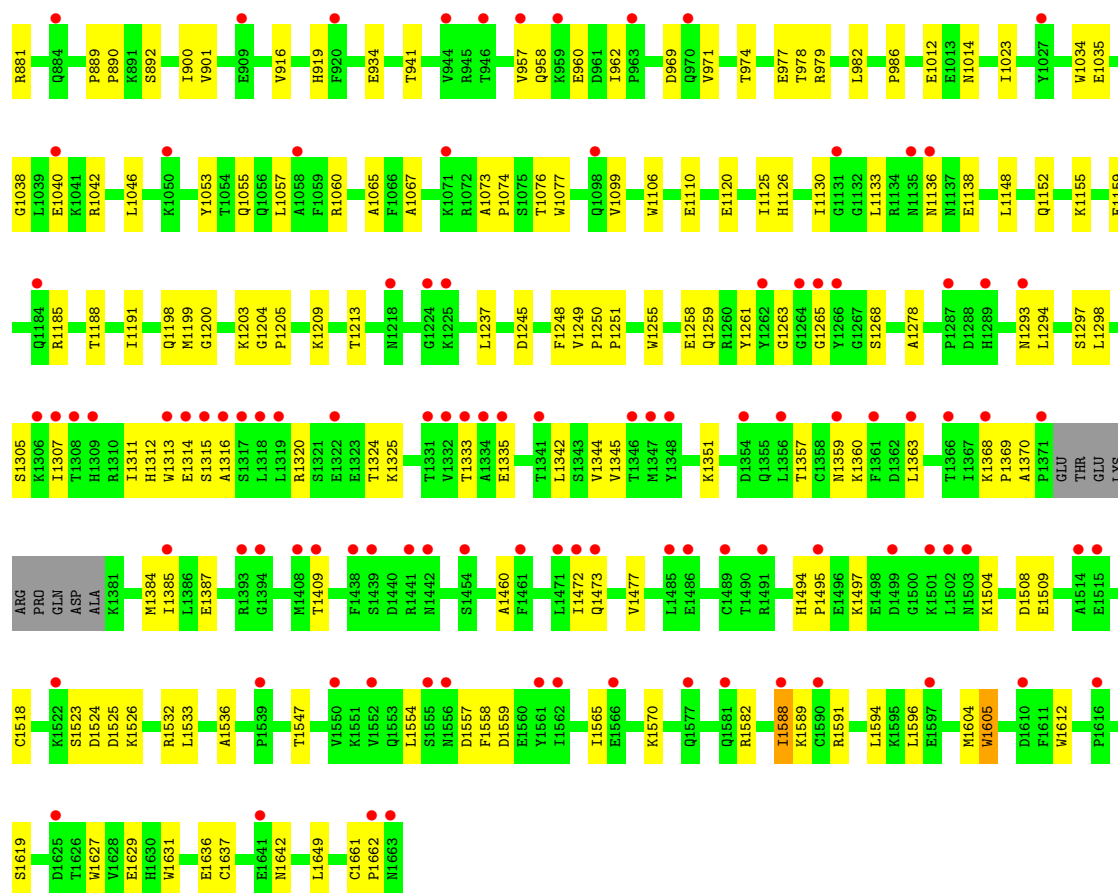


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

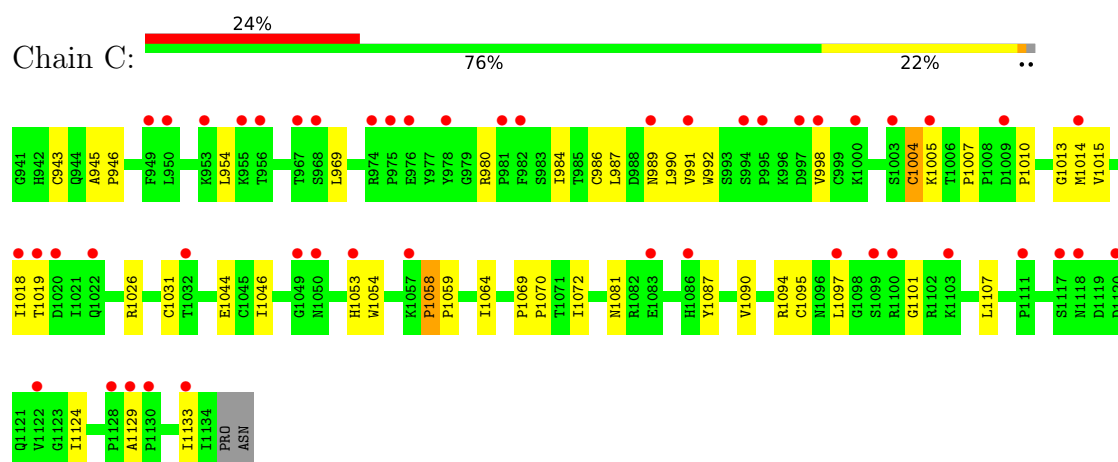


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

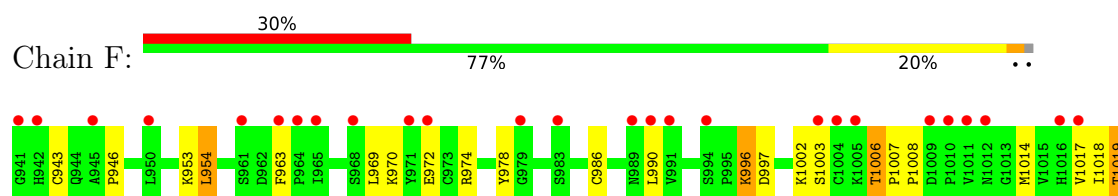


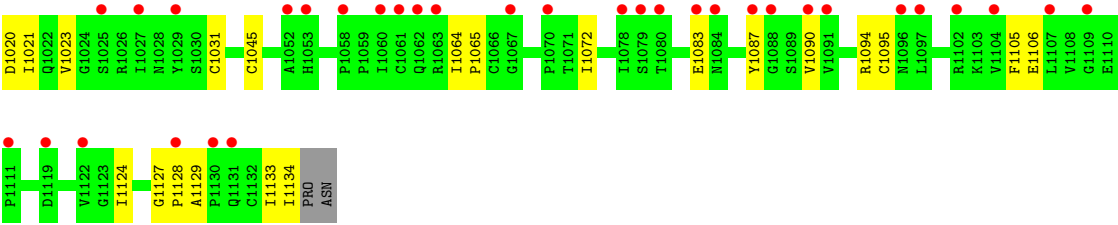


• Molecule 3: COMPLEMENT RECEPTOR TYPE 1



• Molecule 3: COMPLEMENT RECEPTOR TYPE 1





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.251 , 0.291 0.253 , 0.290	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)	0.28 , 103.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.29	0/5108	0.80	1/6940 (0.0%)
1	D	0.29	0/5108	0.78	2/6940 (0.0%)
2	B	0.29	0/7352	0.76	5/9955 (0.1%)
2	E	0.29	0/7352	0.75	3/9955 (0.0%)
3	C	0.38	1/1515 (0.1%)	0.90	3/2066 (0.1%)
3	F	0.38	1/1515 (0.1%)	0.95	7/2066 (0.3%)
All	All	0.30	2/27950 (0.0%)	0.79	21/37922 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1133	ILE	C-N	-6.97	1.23	1.33
3	C	1133	ILE	C-N	-6.97	1.23	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1588	ILE	N-CA-C	-7.50	99.83	109.80
3	C	1058	PRO	CA-C-N	7.45	127.36	120.21
3	C	1058	PRO	C-N-CA	7.45	127.36	120.21
1	D	395	ASP	N-CA-C	6.02	117.84	111.28
2	B	1593	ALA	N-CA-C	-5.98	104.70	112.23
2	B	1250	PRO	N-CA-C	5.85	117.84	110.70
1	D	80	THR	N-CA-C	-5.77	105.90	113.17
3	F	1129	ALA	N-CA-C	5.74	120.04	112.35
3	F	1019	THR	CB-CA-C	-5.62	110.11	116.63
3	F	1105	PHE	CB-CA-C	-5.54	109.20	115.79
2	E	1250	PRO	N-CA-C	5.50	117.41	110.70
2	B	1136	ASN	N-CA-C	5.46	116.97	110.19
3	F	1006	THR	CA-C-N	-5.34	114.88	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1006	THR	C-N-CA	-5.34	114.88	120.38
2	E	1508	ASP	CB-CA-C	-5.32	110.42	116.54
2	B	1508	ASP	CB-CA-C	-5.19	110.57	116.54
3	C	1129	ALA	N-CA-C	5.17	119.28	112.35
2	B	1249	VAL	N-CA-C	5.12	118.50	112.35
1	A	80	THR	N-CA-C	-5.05	106.81	113.17
3	F	996	LYS	CA-C-N	-5.04	113.45	122.32
3	F	996	LYS	C-N-CA	-5.04	113.45	122.32

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	91	0
1	D	5007	0	5063	81	0
2	B	7208	0	7128	90	0
2	E	7208	0	7130	125	0
3	C	1474	0	1407	24	0
3	F	1474	0	1407	23	0
4	A	14	0	13	0	0
4	D	14	0	12	1	0
All	All	27406	0	27224	404	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 (404) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1559:ASP:CG	2:E:1591:ARG:HD3	1.68	1.18
2:E:1554:LEU:HD13	2:E:1591:ARG:NH1	1.57	1.17
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	0.90
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:432:SER:OG	1:A:433:GLU:N	2.27	0.59
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
2:B:971:VAL:O	2:B:974:THR:OG1	2.21	0.58
1:A:162:THR:HG23	3:C:1090:VAL:HG11	1.84	0.58
2:E:971:VAL:O	2:E:974:THR:OG1	2.22	0.57
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
1:D:32:ASN:HB2	1:D:643:GLY:C	2.31	0.56
2:E:1557:ASP:N	2:E:1557:ASP:OD1	2.38	0.56
1:A:83:MET:HE1	1:A:504:GLY:HA2	1.88	0.56
1:A:97:LYS:HB3	1:A:98:SER:HB3	1.88	0.56
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
1:A:263:LYS:HE2	2:B:826:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:1148:LEU:HD21	2:E:1199:MET:HE3	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
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
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
2:E:1384:MET:HE1	2:E:1495:PRO:HB3	1.93	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
1:A:394:GLU:HG2	1:A:396:THR:C	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1495:PRO:HA	2:B:1496:GLU:HG2	1.92	0.51
2:E:1136:ASN:C	2:E:1138:GLU:H	2.17	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
1:A:32:ASN:HB2	1:A:643:GLY:C	2.37	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:261:TYR:HB2	2:B:826:MET:HE2	1.97	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
1:D:72:GLU:HG3	1:D:88:PHE:HB3	1.96	0.46
1:A:45:GLU:HG2	1:A:83:MET:HG3	1.97	0.46
1:A:392:GLN:HA	1:A:393:GLY:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:112:PHE:C	1:D:114:THR:H	2.22	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:135:ASP:OD1	1:D:139:TYR:OH	2.17	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:78:PRO:C	1:D:80:THR:H	2.24	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:D:281:ARG:HH22	1:D:342:GLU:CD	2.25	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
2:E:1524:ASP:HA	2:E:1525:ASP:C	2.42	0.44
1:A:112:PHE:C	1:A:114:THR:H	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1555:SER:OG	2:B:1558:PHE:O	2.28	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
2:B:858:GLN:C	2:B:890:PRO:HG3	2.44	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:889:PRO:O	2:E:892:SER:OG	2.33	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
2:B:1367:ILE:HG13	2:B:1384:MET:HE2	2.00	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:78:PRO:C	1:A:80:THR:H	2.28	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
2:E:1605:TRP:CD1	2:E:1605:TRP:C	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:C:987:LEU:C	3:C:989:ASN:H	2.27	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
1:D:569:GLN:HE22	1:D:581:MET:HE2	1.85	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: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:753:GLU:H	2:E:753:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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	640/645 (99%)	624 (98%)	14 (2%)	2 (0%)	36	65
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%)	48	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	THR
1	A	397	VAL

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	566/567 (100%)	558 (99%)	8 (1%)	59	73
1	D	566/567 (100%)	558 (99%)	8 (1%)	59	73
2	B	798/810 (98%)	791 (99%)	7 (1%)	70	78
2	E	798/810 (98%)	788 (99%)	10 (1%)	61	74
3	C	167/173 (96%)	158 (95%)	9 (5%)	20	49
3	F	167/173 (96%)	158 (95%)	9 (5%)	20	49
All	All	3062/3100 (99%)	3011 (98%)	51 (2%)	53	71

All (51) 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
1	A	200	ASN
1	A	391	VAL
1	A	395	ASP
1	A	428	LYS
1	A	610	LYS
2	B	1023	ILE
2	B	1095	ILE
2	B	1258	GLU
2	B	1318	LEU
2	B	1582	ARG
2	B	1605	TRP
2	B	1637	CYS
3	C	954	LEU
3	C	969	LEU
3	C	986	CYS
3	C	998	VAL
3	C	1004	CYS
3	C	1031	CYS
3	C	1072	ILE
3	C	1107	LEU
3	C	1124	ILE
1	D	32	ASN
1	D	85	ASN
1	D	95	GLU
1	D	265	VAL
1	D	391	VAL
1	D	607	LYS
1	D	610	LYS
1	D	656	GLN
2	E	934	GLU
2	E	1023	ILE
2	E	1258	GLU
2	E	1293	ASN
2	E	1357	THR
2	E	1472	ILE
2	E	1518	CYS
2	E	1582	ARG
2	E	1605	TRP
2	E	1637	CYS
3	F	954	LEU

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Mol	Chain	Res	Type
3	F	969	LEU
3	F	986	CYS
3	F	996	LYS
3	F	997	ASP
3	F	1017	VAL
3	F	1031	CYS
3	F	1072	ILE
3	F	1124	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	185	GLN
1	A	580	GLN
1	A	589	HIS
2	B	774	ASN
2	B	1055	GLN
2	B	1152	GLN
2	B	1277	GLN
2	B	1423	ASN
2	B	1553	GLN
1	D	32	ASN
1	D	126	GLN
1	D	333	HIS
1	D	378	ASN
1	D	454	ASN
1	D	589	HIS
1	D	653	GLN
2	E	1277	GLN
2	E	1312	HIS
2	E	1503	ASN
2	E	1567	GLN
3	F	1012	ASN
3	F	1053	HIS
3	F	1086	HIS

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 oligosaccharides 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	D	1063	1	14,14,15	0.50	0	17,19,21	0.65	0
4	NAG	A	1063	1	14,14,15	0.52	0	17,19,21	1.98	2 (11%)

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	D	1063	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1063	1	1/1/5/7	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(°)	Ideal(°)
4	A	1063	NAG	C1-O5-C5	5.67	119.79	112.19
4	A	1063	NAG	O5-C1-C2	5.07	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, 95th 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%)	0.92	63 (9%)	13 10	75, 118, 176, 230	0
1	D	642/645 (99%)	0.92	64 (9%)	12 10	69, 115, 172, 243	0
2	B	903/915 (98%)	1.31	170 (18%)	3 3	72, 154, 220, 261	0
2	E	903/915 (98%)	1.03	119 (13%)	7 6	65, 134, 196, 234	0
3	C	194/196 (98%)	1.48	48 (24%)	2 1	96, 162, 278, 346	0
3	F	194/196 (98%)	1.72	59 (30%)	1 1	111, 201, 248, 316	0
All	All	3478/3512 (99%)	1.13	523 (15%)	5 5	65, 135, 218, 346	0

All (523) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	70	SER	5.9
1	A	461	LEU	5.3
1	D	396	THR	5.2
1	A	397	VAL	4.8
2	E	1317	SER	4.8
3	C	1118	ASN	4.7
3	F	1060	ILE	4.7
2	B	1611	PHE	4.7
2	E	1136	ASN	4.6
2	B	1527	VAL	4.5
2	B	1318	LEU	4.3
2	E	752	ASP	4.3
2	E	754	ASP	4.3
3	C	1005	LYS	4.3
2	E	1318	LEU	4.2
3	C	1083	GLU	4.2
3	C	981	PRO	4.2
3	C	1117	SER	4.2
3	F	1009	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	994	ALA	4.2
2	B	1166	PRO	4.2
1	A	96	PHE	4.1
2	B	1155	LYS	4.1
2	B	760	ASN	4.0
2	E	1409	THR	4.0
2	B	1176	LEU	4.0
3	F	1058	PRO	3.9
3	F	941	GLY	3.8
2	B	1579	GLY	3.8
2	B	1067	ALA	3.8
1	A	582	THR	3.8
2	B	784	ASN	3.8
2	E	1315	SER	3.8
3	C	1122	VAL	3.7
2	B	1038	GLY	3.7
1	D	71	SER	3.7
1	D	125	LEU	3.7
2	B	1640	GLU	3.7
2	E	1316	ALA	3.7
3	C	1032	THR	3.7
1	A	186	LEU	3.7
3	C	975	PRO	3.7
1	A	395	ASP	3.6
2	B	1317	SER	3.6
1	A	340	GLN	3.6
2	E	1471	LEU	3.6
2	E	1307	ILE	3.6
2	E	1616	PRO	3.5
2	E	1562	ILE	3.5
1	A	398	GLN	3.5
2	B	1141	MET	3.5
3	C	1020	ASP	3.5
2	E	1371	PRO	3.5
1	A	97	LYS	3.5
2	B	1094	ALA	3.5
1	D	438	THR	3.4
2	B	1125	ILE	3.4
2	E	1662	PRO	3.4
1	A	23	SER	3.4
1	A	79	ALA	3.4
3	C	994	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	1114	PRO	3.4
1	A	95	GLU	3.3
2	B	1259	GLN	3.3
2	E	1309	HIS	3.3
2	E	762	VAL	3.3
3	C	1129	ALA	3.3
1	D	393	GLY	3.3
2	B	1545	TYR	3.3
2	B	1083	VAL	3.3
2	E	1058	ALA	3.3
3	F	965	ILE	3.3
3	C	995	PRO	3.2
1	A	588	ASP	3.2
3	F	1122	VAL	3.2
2	E	1438	PHE	3.2
3	C	1014	MET	3.2
3	C	1133	ILE	3.2
2	E	1368	LYS	3.2
2	B	1156	ASP	3.2
2	B	1588	ILE	3.2
2	E	1663	ASN	3.2
1	D	520	SER	3.1
3	F	945	ALA	3.1
1	A	337	ASP	3.1
1	D	403	GLY	3.1
2	B	1440	ASP	3.1
3	C	950	LEU	3.1
3	C	1128	PRO	3.1
1	A	69	LEU	3.1
2	B	1046	LEU	3.1
2	E	1590	CYS	3.1
2	B	1062	PRO	3.1
1	A	70	SER	3.1
2	B	1148	LEU	3.1
3	F	1130	PRO	3.1
1	D	95	GLU	3.0
2	B	934	GLU	3.0
2	E	1486	GLU	3.0
3	C	1130	PRO	3.0
3	F	964	PRO	3.0
3	C	953	LYS	3.0
2	E	846	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	1010	PRO	3.0
2	B	1596	LEU	3.0
2	E	1503	ASN	3.0
3	F	979	GLY	3.0
2	B	1547	THR	3.0
2	B	1205	PRO	3.0
3	F	1128	PRO	3.0
2	B	1571	SER	3.0
1	D	94	ARG	3.0
2	B	997	ALA	3.0
2	B	1058	ALA	3.0
1	D	128	GLY	3.0
3	F	1104	VAL	3.0
2	B	1633	GLU	3.0
2	B	1053	TYR	3.0
2	B	1026	HIS	3.0
2	E	1135	ASN	3.0
3	F	1084	ASN	3.0
2	B	1202	LEU	2.9
1	A	427	LYS	2.9
1	A	520	SER	2.9
1	A	558	SER	2.9
2	B	1573	SER	2.9
3	F	1011	VAL	2.9
2	B	1607	LEU	2.9
1	A	399	SER	2.9
2	E	861	LYS	2.9
2	B	1316	ALA	2.9
1	D	39	GLU	2.9
2	B	917	TYR	2.9
2	E	1385	ILE	2.9
2	B	1212	THR	2.9
3	F	991	VAL	2.9
2	B	1151	LEU	2.9
2	E	1319	LEU	2.9
2	B	1153	GLU	2.8
2	B	1458	CYS	2.8
2	B	1355	GLN	2.8
3	C	1022	GLN	2.8
3	F	1131	GLN	2.8
1	D	430	GLU	2.8
2	E	1555	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	974	ARG	2.8
2	B	1070	VAL	2.8
1	D	404	ASP	2.8
2	E	1333	THR	2.8
3	F	1027	ILE	2.8
2	B	1101	CYS	2.8
3	C	1086	HIS	2.8
1	D	213	SER	2.8
2	B	995	VAL	2.8
3	F	1005	LYS	2.8
1	D	509	GLU	2.8
2	B	1529	LEU	2.8
3	F	1080	THR	2.8
1	D	397	VAL	2.8
2	B	1104	VAL	2.8
3	F	1070	PRO	2.8
2	B	1502	LEU	2.8
3	F	1090	VAL	2.7
1	D	431	LEU	2.7
1	A	98	SER	2.7
1	A	231	SER	2.7
1	A	334	SER	2.7
2	B	1146	PHE	2.7
3	F	994	SER	2.7
2	E	1394	GLY	2.7
3	F	1109	GLY	2.7
1	D	126	GLN	2.7
2	B	1005	VAL	2.7
2	B	1090	VAL	2.7
3	F	1062	GLN	2.7
3	F	1097	LEU	2.7
2	E	920	PHE	2.7
2	E	1265	GLY	2.7
3	F	1088	GLY	2.7
2	B	861	LYS	2.7
2	B	1522	LYS	2.7
2	B	1635	ASP	2.7
3	F	1052	ALA	2.7
2	B	1025	VAL	2.7
2	B	1162	VAL	2.7
1	A	574	GLN	2.7
2	B	1248	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	1049	GLY	2.7
2	B	985	THR	2.7
1	A	323	SER	2.7
2	B	1001	LYS	2.7
3	F	961	SER	2.7
1	D	395	ASP	2.7
2	B	923	ASP	2.7
2	B	1136	ASN	2.7
2	B	1143	LEU	2.7
2	E	1334	ALA	2.7
2	B	1632	PRO	2.6
2	B	1041	LYS	2.6
2	B	895	SER	2.6
1	D	96	PHE	2.6
2	E	1287	PRO	2.6
2	E	1408	MET	2.6
2	E	753	GLU	2.6
2	B	1068	ALA	2.6
2	B	798	SER	2.6
2	E	959	LYS	2.6
2	E	1441	ARG	2.6
2	E	1442	ASN	2.6
2	B	1554	LEU	2.6
2	B	1139	LYS	2.6
3	F	1102	ARG	2.6
2	B	1228	TYR	2.6
2	E	1472	ILE	2.6
1	A	518	PRO	2.6
2	E	884	GLN	2.6
2	B	984	GLY	2.6
1	A	586	GLU	2.6
2	B	1319	LEU	2.6
1	D	544	ARG	2.6
2	B	1570	LYS	2.6
1	A	338	MET	2.6
2	B	1539	PRO	2.6
1	D	461	LEU	2.6
3	C	1097	LEU	2.6
2	B	1103	ALA	2.6
2	E	794	PHE	2.5
2	B	1100	LEU	2.5
3	C	1100	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	1063	ARG	2.5
2	B	1030	GLU	2.5
2	B	1565	ILE	2.5
2	E	1361	PHE	2.5
1	D	353	TYR	2.5
3	F	1004	CYS	2.5
2	E	1264	GLY	2.5
3	F	968	SER	2.5
3	F	1079	SER	2.5
1	A	540	ALA	2.5
2	B	1128	GLU	2.5
3	C	1009	ASP	2.5
1	A	462	ARG	2.5
2	E	1071	LYS	2.5
3	F	1067	GLY	2.5
2	B	884	GLN	2.5
2	E	874	SER	2.5
3	C	968	SER	2.5
2	E	1514	ALA	2.5
2	E	1515	GLU	2.5
2	E	1354	ASP	2.5
2	E	1588	ILE	2.5
2	E	1610	ASP	2.5
1	A	396	THR	2.5
1	D	499	ARG	2.5
2	B	1183	LEU	2.5
2	B	1471	LEU	2.5
2	E	1501	LYS	2.5
2	E	946	THR	2.5
1	A	154	HIS	2.5
1	A	113	GLY	2.5
3	F	1025	SER	2.4
2	E	1566	GLU	2.4
1	D	166	ASN	2.4
1	D	612	THR	2.4
3	F	1119	ASP	2.4
2	E	1131	GLY	2.4
1	A	581	MET	2.4
2	B	1015	MET	2.4
2	B	1158	CYS	2.4
2	E	873	CYS	2.4
2	E	1454	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	949	PHE	2.4
2	B	1165	LEU	2.4
1	A	52	ASP	2.4
2	B	878	THR	2.4
2	B	1179	ASN	2.4
2	B	1442	ASN	2.4
2	B	1556	ASN	2.4
2	E	1359	ASN	2.4
2	E	1366	THR	2.4
3	C	998	VAL	2.4
3	F	1053	HIS	2.4
3	F	1087	TYR	2.4
1	D	586	GLU	2.4
2	B	1066	PHE	2.4
1	D	336	SER	2.4
2	B	1661	CYS	2.4
2	E	1346	THR	2.4
2	E	1499	ASP	2.4
2	E	1552	VAL	2.4
2	B	1243	LEU	2.4
2	E	1314	GLU	2.4
1	D	536	THR	2.4
2	B	1371	PRO	2.4
2	B	1612	TRP	2.4
3	C	956	THR	2.4
3	F	989	ASN	2.4
1	D	52	ASP	2.4
2	E	811	ASP	2.4
1	A	538	ILE	2.4
1	D	434	ALA	2.4
2	B	1157	ILE	2.4
2	B	783	LYS	2.4
2	B	1436	LYS	2.4
2	B	1645	GLN	2.4
3	C	982	PHE	2.4
1	D	67	LEU	2.4
3	F	950	LEU	2.4
2	E	1439	SER	2.4
2	B	1616	PRO	2.4
3	F	1091	VAL	2.4
2	B	1394	GLY	2.3
2	E	1331	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	462	ARG	2.3
3	C	978	TYR	2.3
1	D	357	PHE	2.3
2	B	1530	GLU	2.3
2	E	1332	VAL	2.3
1	D	23	SER	2.3
1	D	383	PRO	2.3
2	B	1034	TRP	2.3
2	B	1168	SER	2.3
1	A	235	ILE	2.3
3	F	1016	HIS	2.3
2	B	1482	TYR	2.3
2	B	1567	GLN	2.3
2	E	970	GLN	2.3
2	E	1322	GLU	2.3
2	B	959	LYS	2.3
1	D	158	PRO	2.3
3	F	1111	PRO	2.3
2	B	1116	GLY	2.3
2	B	1523	SER	2.3
1	D	373	MET	2.3
2	B	1563	MET	2.3
3	F	942	HIS	2.3
2	E	1556	ASN	2.3
2	E	1461	PHE	2.3
2	B	1557	ASP	2.3
2	E	1577	GLN	2.3
1	A	237	GLU	2.3
1	A	240	GLU	2.3
1	D	659	GLU	2.3
1	A	336	SER	2.3
3	C	1003	SER	2.3
2	B	1257	ASN	2.3
2	E	1293	ASN	2.3
1	D	392	GLN	2.3
2	E	777	ASP	2.3
2	B	1600	LYS	2.3
3	C	1103	LYS	2.3
2	B	766	GLU	2.3
3	C	976	GLU	2.3
2	E	1347	MET	2.3
3	F	990	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	1289	HIS	2.3
1	D	567	SER	2.3
2	E	810	SER	2.3
3	C	989	ASN	2.3
3	C	991	VAL	2.3
3	C	997	ASP	2.3
3	C	1120	ASP	2.3
2	B	1263	GLY	2.2
2	E	1485	LEU	2.2
1	A	612	THR	2.2
1	D	647	THR	2.2
2	E	1341	THR	2.2
1	A	71	SER	2.2
1	D	502	LYS	2.2
2	B	1217	LYS	2.2
3	F	1029	TYR	2.2
2	E	863	ARG	2.2
1	A	280	GLN	2.2
2	E	944	VAL	2.2
2	E	1625	ASP	2.2
1	D	173	ILE	2.2
2	B	781	PRO	2.2
2	B	1057	LEU	2.2
2	B	1073	ALA	2.2
2	B	1129	MET	2.2
2	E	1356	LEU	2.2
1	D	385	TYR	2.2
2	B	765	SER	2.2
3	F	983	SER	2.2
2	E	1218	ASN	2.2
1	A	171	GLU	2.2
1	A	331	ILE	2.2
1	A	83	MET	2.2
1	A	503	ALA	2.2
2	B	1587	PRO	2.2
3	C	1111	PRO	2.2
2	E	1313	TRP	2.2
2	E	1491	ARG	2.2
2	E	1308	THR	2.2
2	E	1262	TYR	2.2
1	D	417	GLN	2.2
1	D	429	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	1473	GLN	2.2
2	E	1581	GLN	2.2
2	B	860	LEU	2.2
2	B	975	GLU	2.2
3	F	1107	LEU	2.2
3	F	1061	CYS	2.2
2	B	1029	ASP	2.2
2	B	1069	PHE	2.2
2	B	1210	PHE	2.2
2	E	1393	ARG	2.2
3	F	1017	VAL	2.2
2	B	1043	GLN	2.2
2	B	1356	LEU	2.2
1	A	99	GLU	2.2
2	B	1177	GLU	2.2
2	B	1197	ALA	2.2
2	E	1040	GLU	2.2
2	E	1335	GLU	2.2
2	E	1522	LYS	2.2
3	C	955	LYS	2.2
3	F	1012	ASN	2.2
3	F	1096	ASN	2.2
2	B	1009	GLY	2.2
1	A	256	THR	2.1
1	D	398	GLN	2.1
2	B	1227	LEU	2.1
2	B	1533	LEU	2.1
2	E	1098	GLN	2.1
2	E	1184	GLN	2.1
2	E	1363	LEU	2.1
1	D	97	LYS	2.1
2	E	1225	LYS	2.1
1	D	568	GLY	2.1
2	B	1200	GLY	2.1
2	B	939	ASN	2.1
3	F	963	PHE	2.1
2	B	996	ASP	2.1
2	E	957	VAL	2.1
2	B	1023	ILE	2.1
2	E	755	ILE	2.1
1	A	67	LEU	2.1
2	B	1033	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1593	ALA	2.1
1	D	432	SER	2.1
2	B	1123	PRO	2.1
2	B	1575	GLU	2.1
2	E	843	GLU	2.1
3	C	1099	SER	2.1
3	C	1050	ASN	2.1
1	A	86	VAL	2.1
1	D	73	LYS	2.1
1	D	209	TYR	2.1
2	B	1084	LYS	2.1
3	C	967	THR	2.1
1	D	540	ALA	2.1
3	F	972	GLU	2.1
3	F	1083	GLU	2.1
1	A	38	SER	2.1
2	B	1150	SER	2.1
2	B	1558	PHE	2.1
3	F	1003	SER	2.1
1	A	85	ASN	2.1
1	D	93	ASN	2.1
1	D	391	VAL	2.1
1	D	371	ASP	2.1
1	D	457	HIS	2.1
2	B	1595	LYS	2.1
2	B	790	LEU	2.1
1	A	107	THR	2.1
1	A	426	THR	2.1
1	A	463	THR	2.1
1	D	463	THR	2.1
2	B	753	GLU	2.1
2	E	1495	PRO	2.1
2	B	1439	SER	2.1
2	B	1099	VAL	2.1
2	B	1230	VAL	2.1
1	D	85	ASN	2.1
2	B	1163	ASN	2.1
3	C	1000	LYS	2.1
1	D	186	LEU	2.1
2	B	752	ASP	2.1
2	B	1341	THR	2.1
2	B	1366	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	1027	TYR	2.1
2	B	1145	ALA	2.1
2	B	1154	ALA	2.1
1	A	321	GLY	2.1
1	D	543	GLN	2.1
2	B	1438	PHE	2.1
2	E	1539	PRO	2.1
2	E	1641	GLU	2.1
1	A	236	VAL	2.0
1	A	391	VAL	2.0
2	E	1050	LYS	2.0
3	C	1057	LYS	2.0
3	F	1078	ILE	2.0
2	B	754	ASP	2.0
2	E	1266	TYR	2.0
2	E	1348	TYR	2.0
2	E	1561	TYR	2.0
3	C	1019	THR	2.0
3	F	971	TYR	2.0
2	E	1489	CYS	2.0
2	B	1277	GLN	2.0
2	E	1224	GLY	2.0
1	A	230	PRO	2.0
1	A	607	LYS	2.0
2	B	1036	LYS	2.0
2	E	909	GLU	2.0
1	A	546	VAL	2.0
2	E	817	VAL	2.0
2	E	1502	LEU	2.0
1	A	313	ASN	2.0
2	B	1199	MET	2.0
3	C	1053	HIS	2.0
2	B	1027	TYR	2.0
2	B	1357	THR	2.0
2	B	1399	THR	2.0
2	B	1295	ASP	2.0
2	E	963	PRO	2.0
2	E	1306	LYS	2.0
1	D	43	VAL	2.0
2	E	1550	VAL	2.0
2	E	1597	GLU	2.0
3	C	1018	ILE	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
4	NAG	A	1063	14/15	0.68	0.20	106,127,145,146	0
4	NAG	D	1063	14/15	0.77	0.17	87,134,158,164	0

6.5 Other polymers [i](#)

There are no such residues in this entry.