



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:50 PM GMT

PDB ID : 4WRM
Title : Structure of the human CSF-1:CSF-1R complex
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Deposited on : 2014-10-24
Resolution : 6.85 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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

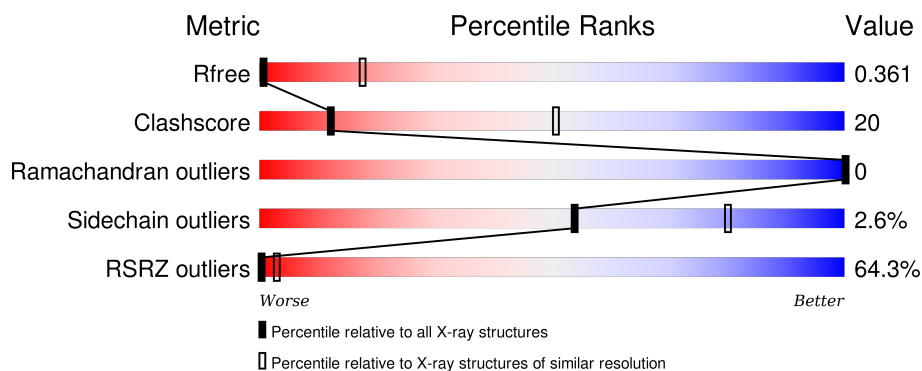
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.85 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}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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. 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	493	
2	B	170	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4524 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 Macrophage colony-stimulating factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3422	2183	589	636	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	THR	-	expression tag	UNP P07333
A	506	LYS	-	expression tag	UNP P07333
A	507	HIS	-	expression tag	UNP P07333
A	508	HIS	-	expression tag	UNP P07333
A	509	HIS	-	expression tag	UNP P07333
A	510	HIS	-	expression tag	UNP P07333
A	511	HIS	-	expression tag	UNP P07333
A	512	HIS	-	expression tag	UNP P07333

- Molecule 2 is a protein called Macrophage colony-stimulating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	141	1102	691	185	215	11	0	0	0

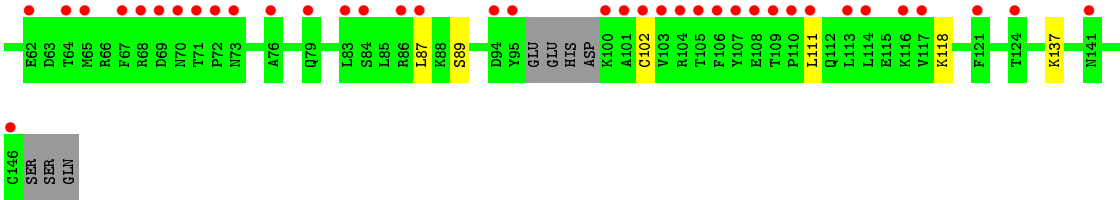
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP P09603
B	-19	GLY	-	expression tag	UNP P09603
B	-18	SER	-	expression tag	UNP P09603
B	-17	SER	-	expression tag	UNP P09603
B	-16	HIS	-	expression tag	UNP P09603
B	-15	HIS	-	expression tag	UNP P09603
B	-14	HIS	-	expression tag	UNP P09603
B	-13	HIS	-	expression tag	UNP P09603

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP P09603
B	-11	HIS	-	expression tag	UNP P09603
B	-10	SER	-	expression tag	UNP P09603
B	-9	SER	-	expression tag	UNP P09603
B	-8	GLY	-	expression tag	UNP P09603
B	-7	LEU	-	expression tag	UNP P09603
B	-6	VAL	-	expression tag	UNP P09603
B	-5	PRO	-	expression tag	UNP P09603
B	-4	ARG	-	expression tag	UNP P09603
B	-3	GLY	-	expression tag	UNP P09603
B	-2	SER	-	expression tag	UNP P09603
B	-1	HIS	-	expression tag	UNP P09603
B	0	MET	-	expression tag	UNP P09603



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	281.47Å 281.47Å 91.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.75 – 6.85 48.75 – 6.80	Depositor EDS
% Data completeness (in resolution range)	82.7 (48.75-6.85) 99.9 (48.75-6.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1685)	Depositor
R, R_{free}	0.326 , 0.359 0.342 , 0.361	Depositor DCC
R_{free} test set	384 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	446.7	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 560.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 3953 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	4524	wwPDB-VP
Average B, all atoms (Å ²)	313.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/3509	0.61	0/4788
2	B	0.25	0/1118	0.39	0/1513
All	All	0.40	0/4627	0.56	0/6301

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 [i](#)

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	3422	0	3286	163	3
2	B	1102	0	1034	13	0
All	All	4524	0	4320	175	3

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 20.

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:CG2	1:A:298:SER:CA	1.74	1.65
1:A:28:PRO:O	1:A:159:TRP:CZ2	1.64	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HD13	1:A:299:ALA:N	1.18	1.44
1:A:215:ILE:CG2	1:A:298:SER:HA	1.32	1.42
1:A:215:ILE:CD1	1:A:299:ALA:HA	1.51	1.40
1:A:215:ILE:CD1	1:A:299:ALA:CA	2.00	1.39
1:A:215:ILE:HG23	1:A:298:SER:N	1.33	1.38
1:A:338:TYR:CE1	1:A:340:GLY:HA3	1.61	1.36
1:A:215:ILE:HG23	1:A:298:SER:CA	1.39	1.35
1:A:104:PRO:O	1:A:105:ALA:HB3	1.19	1.33
1:A:214:ARG:NH1	1:A:328:TYR:OH	1.62	1.29
1:A:338:TYR:CZ	1:A:340:GLY:HA3	1.68	1.27
1:A:215:ILE:HD11	1:A:299:ALA:CA	1.65	1.20
1:A:215:ILE:CD1	1:A:299:ALA:N	2.03	1.19
1:A:342:PHE:CD2	1:A:374:SER:HA	1.78	1.18
1:A:215:ILE:HD13	1:A:299:ALA:CA	1.65	1.17
1:A:215:ILE:CG2	1:A:298:SER:C	2.16	1.13
1:A:79:THR:HB	1:A:109:ASN:HD22	1.00	1.12
1:A:215:ILE:HG21	1:A:298:SER:CA	1.55	1.11
1:A:79:THR:HB	1:A:109:ASN:ND2	1.68	1.08
1:A:28:PRO:O	1:A:159:TRP:CH2	2.10	1.05
1:A:104:PRO:O	1:A:105:ALA:CB	2.06	1.04
1:A:98:HIS:HB2	1:A:159:TRP:CD2	1.92	1.03
1:A:338:TYR:CZ	1:A:340:GLY:CA	2.40	1.03
1:A:312:GLU:OE1	1:A:424:TYR:HD2	1.41	1.03
1:A:312:GLU:OE1	1:A:424:TYR:CD2	2.11	1.02
1:A:104:PRO:C	1:A:106:ARG:HG2	1.83	0.99
1:A:215:ILE:HG23	1:A:298:SER:C	1.81	0.94
1:A:215:ILE:HG21	1:A:298:SER:HA	0.93	0.93
1:A:215:ILE:CG2	1:A:298:SER:N	2.11	0.93
1:A:28:PRO:C	1:A:159:TRP:HZ2	1.72	0.92
1:A:215:ILE:HD13	1:A:299:ALA:H	1.32	0.91
1:A:347:PRO:HA	1:A:350:LYS:HD3	1.50	0.90
1:A:338:TYR:CE1	1:A:340:GLY:CA	2.51	0.90
1:A:338:TYR:CE2	1:A:340:GLY:O	2.25	0.88
1:A:104:PRO:O	1:A:106:ARG:HG2	1.74	0.88
1:A:103:ASP:O	1:A:106:ARG:HB2	1.72	0.88
1:A:215:ILE:HG22	1:A:298:SER:HA	1.55	0.88
1:A:100:TYR:HD1	1:A:130:THR:HA	1.39	0.87
2:B:3:VAL:HG22	2:B:89:SER:O	1.73	0.87
1:A:342:PHE:CE1	1:A:374:SER:HB3	2.10	0.86
1:A:215:ILE:HG21	1:A:298:SER:C	1.88	0.85
1:A:29:GLU:OE2	1:A:132:PRO:HG3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HD11	1:A:299:ALA:HA	0.86	0.84
1:A:214:ARG:NH1	1:A:328:TYR:CZ	2.31	0.84
1:A:28:PRO:O	1:A:159:TRP:HZ2	1.20	0.83
1:A:338:TYR:HE2	1:A:342:PHE:O	1.60	0.82
1:A:239:HIS:CD2	1:A:240:ASN:OD1	2.34	0.81
1:A:342:PHE:CG	1:A:374:SER:HA	2.16	0.81
1:A:100:TYR:CD1	1:A:130:THR:HA	2.15	0.81
1:A:463:PHE:CD2	1:A:463:PHE:O	2.35	0.80
1:A:215:ILE:HG12	1:A:298:SER:O	1.84	0.78
1:A:90:PRO:O	1:A:91:LEU:HB2	1.83	0.78
1:A:342:PHE:CD1	1:A:374:SER:HB3	2.18	0.77
1:A:342:PHE:CD1	1:A:374:SER:CB	2.67	0.76
1:A:214:ARG:NH1	1:A:328:TYR:CE1	2.55	0.74
1:A:79:THR:CB	1:A:109:ASN:HD22	1.90	0.73
1:A:215:ILE:CD1	1:A:299:ALA:CB	2.67	0.72
1:A:338:TYR:CZ	1:A:340:GLY:C	2.63	0.71
1:A:463:PHE:CG	1:A:463:PHE:O	2.43	0.71
1:A:406:VAL:HA	1:A:419:CYS:HA	1.72	0.70
1:A:342:PHE:CE2	1:A:374:SER:HA	2.28	0.69
1:A:215:ILE:CG1	1:A:298:SER:C	2.60	0.69
1:A:407:ILE:O	1:A:418:LEU:N	2.28	0.66
1:A:98:HIS:HB2	1:A:159:TRP:CE2	2.30	0.66
1:A:405:SER:O	1:A:420:ALA:N	2.27	0.65
1:A:312:GLU:OE1	1:A:424:TYR:CE2	2.50	0.65
1:A:215:ILE:HG12	1:A:298:SER:C	2.17	0.65
1:A:400:TYR:HB2	1:A:423:GLY:HA2	1.79	0.65
1:A:432:LEU:N	1:A:484:GLU:O	2.19	0.64
1:A:419:CYS:N	1:A:470:SER:O	2.25	0.64
1:A:430:THR:N	1:A:486:ARG:O	2.28	0.64
1:A:342:PHE:CG	1:A:374:SER:CA	2.81	0.64
1:A:342:PHE:HB3	1:A:374:SER:O	1.96	0.64
1:A:89:ASP:OD1	1:A:90:PRO:HD2	1.98	0.64
1:A:430:THR:HB	1:A:486:ARG:HB2	1.79	0.63
1:A:407:ILE:N	1:A:418:LEU:O	2.25	0.62
1:A:90:PRO:O	1:A:91:LEU:CB	2.43	0.62
1:A:424:TYR:CD1	1:A:425:PRO:HA	2.34	0.62
1:A:419:CYS:O	1:A:470:SER:N	2.22	0.62
1:A:428:ASN:HB3	1:A:453:PRO:HA	1.82	0.62
1:A:29:GLU:OE2	1:A:132:PRO:CG	2.47	0.61
1:A:98:HIS:CB	1:A:159:TRP:CE2	2.84	0.61
1:A:98:HIS:CE1	1:A:159:TRP:HA	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:OD1	1:A:240:ASN:N	2.33	0.60
1:A:215:ILE:HD13	1:A:298:SER:C	2.13	0.60
1:A:338:TYR:CE2	1:A:342:PHE:O	2.50	0.60
1:A:342:PHE:CB	1:A:374:SER:O	2.50	0.60
1:A:408:TRP:HB2	1:A:417:LEU:HD23	1.84	0.60
1:A:28:PRO:C	1:A:159:TRP:CZ2	2.54	0.60
1:A:215:ILE:HD11	1:A:299:ALA:CB	2.31	0.59
1:A:98:HIS:CE1	1:A:159:TRP:O	2.54	0.59
1:A:89:ASP:OD1	1:A:90:PRO:CD	2.51	0.58
1:A:430:THR:O	1:A:486:ARG:N	2.29	0.58
1:A:215:ILE:HG21	1:A:299:ALA:N	2.17	0.58
1:A:104:PRO:C	1:A:105:ALA:HB3	2.16	0.58
1:A:323:VAL:HG21	1:A:381:PHE:CD2	2.39	0.58
1:A:98:HIS:CB	1:A:159:TRP:CD2	2.77	0.58
1:A:399:ARG:HD2	1:A:491:VAL:HG22	1.84	0.58
1:A:324:MET:HG3	1:A:363:THR:HG22	1.87	0.56
1:A:98:HIS:HB2	1:A:159:TRP:CE3	2.39	0.56
1:A:428:ASN:CB	1:A:453:PRO:HA	2.36	0.56
1:A:338:TYR:CE2	1:A:340:GLY:C	2.78	0.56
1:A:459:SER:HB2	1:A:467:THR:OG1	2.05	0.56
1:A:215:ILE:CD1	1:A:298:SER:C	2.72	0.55
1:A:407:ILE:HG13	1:A:418:LEU:HB3	1.88	0.55
1:A:80:GLY:HA2	1:A:128:LEU:HD13	1.88	0.55
1:A:458:LEU:HD12	1:A:469:GLN:HB2	1.88	0.54
1:A:29:GLU:OE2	1:A:132:PRO:HB3	2.07	0.54
1:A:342:PHE:CG	1:A:374:SER:CB	2.90	0.54
1:A:215:ILE:HD13	1:A:299:ALA:CB	2.33	0.54
1:A:432:LEU:O	1:A:484:GLU:HB3	2.07	0.53
1:A:421:ALA:O	1:A:468:VAL:HG22	2.08	0.53
1:A:336:TRP:CD1	1:A:351:LEU:HD13	2.43	0.53
1:A:29:GLU:OE2	1:A:132:PRO:CB	2.56	0.53
1:A:342:PHE:CD1	1:A:374:SER:HB2	2.44	0.52
1:A:486:ARG:HA	1:A:495:SER:HA	1.91	0.52
1:A:215:ILE:CD1	1:A:299:ALA:HB2	2.39	0.52
1:A:35:GLY:HA2	1:A:73:ASN:OD1	2.10	0.52
1:A:431:TRP:O	1:A:449:VAL:HG13	2.10	0.52
1:A:332:GLN:HG2	1:A:385:ASN:HA	1.92	0.51
1:A:406:VAL:HG13	1:A:431:TRP:HH2	1.75	0.51
1:A:224:CYS:HB2	1:A:237:LEU:HD13	1.92	0.50
2:B:4:SER:OG	2:B:6:TYR:CD2	2.64	0.50
1:A:100:TYR:CD1	1:A:130:THR:CA	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PRO:HB2	1:A:287:HIS:HB2	1.93	0.50
1:A:98:HIS:HB2	1:A:159:TRP:CG	2.43	0.50
1:A:488:HIS:HA	1:A:492:GLY:O	2.13	0.49
2:B:4:SER:HG	2:B:6:TYR:HD2	1.60	0.49
1:A:98:HIS:HB3	1:A:159:TRP:CE2	2.49	0.48
2:B:3:VAL:CG2	2:B:89:SER:O	2.56	0.47
1:A:431:TRP:CZ3	1:A:485:CYS:HB2	2.49	0.47
1:A:103:ASP:O	1:A:106:ARG:CB	2.53	0.47
1:A:424:TYR:HD1	1:A:466:VAL:HG21	1.79	0.46
1:A:408:TRP:HA	1:A:417:LEU:HA	1.98	0.46
1:A:400:TYR:CD2	1:A:465:LYS:HD3	2.50	0.46
1:A:150:ARG:HG2	1:A:151:HIS:CD2	2.50	0.46
1:A:205:LEU:HD13	1:A:289:THR:HG22	1.96	0.46
1:A:296:VAL:O	1:A:298:SER:N	2.49	0.46
1:A:485:CYS:O	1:A:495:SER:HA	2.15	0.46
1:A:424:TYR:HD1	1:A:466:VAL:CG2	2.28	0.46
2:B:2:GLU:HB3	2:B:89:SER:HB2	1.97	0.46
2:B:10:MET:HE3	2:B:87:LEU:HD23	1.97	0.46
1:A:63:ASP:OD1	1:A:64:GLY:N	2.49	0.46
1:A:484:GLU:HG3	1:A:495:SER:OG	2.16	0.45
1:A:89:ASP:HA	1:A:90:PRO:HD3	1.84	0.45
2:B:19:LEU:HD13	2:B:118:LYS:HA	1.99	0.45
1:A:24:GLU:OE1	1:A:41:ARG:NH1	2.44	0.44
1:A:239:HIS:CG	1:A:240:ASN:OD1	2.71	0.44
1:A:157:SER:HA	1:A:158:PRO:HD3	1.87	0.44
1:A:405:SER:O	1:A:419:CYS:HA	2.18	0.43
1:A:303:LEU:HD13	1:A:390:ARG:HB2	2.01	0.43
1:A:486:ARG:HA	1:A:494:GLY:O	2.18	0.43
1:A:240:ASN:HB2	1:A:241:ASN:H	1.62	0.43
1:A:98:HIS:HE1	1:A:159:TRP:O	2.02	0.43
2:B:43:LEU:HD11	2:B:102:CYS:SG	2.59	0.43
1:A:104:PRO:C	1:A:106:ARG:CG	2.71	0.43
1:A:278:CYS:N	1:A:289:THR:O	2.44	0.43
1:A:313:VAL:HG13	1:A:317:GLU:HB2	2.00	0.43
2:B:26:GLN:HB2	2:B:111:LEU:HD21	2.00	0.42
1:A:76:PHE:O	1:A:109:ASN:ND2	2.52	0.42
1:A:239:HIS:C	1:A:240:ASN:OD1	2.58	0.42
1:A:404:VAL:HG13	1:A:419:CYS:SG	2.59	0.42
1:A:432:LEU:O	1:A:484:GLU:N	2.40	0.42
1:A:98:HIS:CB	1:A:159:TRP:CG	3.02	0.42
1:A:402:PRO:HA	1:A:422:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:HA	1:A:54:PRO:HD3	1.97	0.41
1:A:231:VAL:HG11	2:B:10:MET:SD	2.61	0.41
2:B:2:GLU:HG2	2:B:2:GLU:O	2.20	0.41
1:A:406:VAL:HA	1:A:418:LEU:O	2.21	0.41
2:B:38:VAL:HG23	2:B:43:LEU:HD13	2.02	0.41
1:A:146:ARG:H	1:A:146:ARG:HG2	1.62	0.41
2:B:137:LYS:HE3	2:B:137:LYS:HB2	1.92	0.41
1:A:135:GLU:O	1:A:138:VAL:HG22	2.21	0.41
1:A:428:ASN:OD1	1:A:488:HIS:O	2.40	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:NH2	1:A:375:GLU:OE2[9_554]	1.67	0.53
1:A:370:ARG:NH1	1:A:375:GLU:OE1[9_554]	2.11	0.09
1:A:91:LEU:CD2	1:A:452:ASP:OD1[12_565]	2.11	0.09

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	423/493 (86%)	406 (96%)	17 (4%)	0	100	100
2	B	137/170 (81%)	132 (96%)	5 (4%)	0	100	100
All	All	560/663 (84%)	538 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	372/429 (87%)	359 (96%)	13 (4%)	43	74
2	B	122/160 (76%)	122 (100%)	0	100	100
All	All	494/589 (84%)	481 (97%)	13 (3%)	54	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ARG
1	A	240	ASN
1	A	324	MET
1	A	326	GLU
1	A	332	GLN
1	A	342	PHE
1	A	346	GLN
1	A	351	LEU
1	A	450	TRP
1	A	458	LEU
1	A	460	GLN
1	A	461	GLU
1	A	498	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	239	HIS
1	A	320	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	399:ARG	C	400:TYR	N	4.38
1	A	104:PRO	C	105:ALA	N	4.10

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	445/493 (90%)	4.48	307 (68%) 0 3	216, 314, 410, 458	0
2	B	141/170 (82%)	2.54	70 (49%) 0 4	213, 290, 416, 477	0
All	All	586/663 (88%)	4.01	377 (64%) 0 3	213, 307, 411, 477	0

All (377) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ALA	19.0
1	A	295	VAL	18.1
1	A	268	VAL	18.0
1	A	203	PRO	17.3
1	A	204	ALA	16.3
1	A	235	VAL	15.4
1	A	269	ASP	15.2
1	A	265	LEU	14.6
1	A	222	ILE	12.7
1	A	230	ASP	12.6
1	A	290	SER	12.6
1	A	434	CYS	12.5
1	A	272	HIS	12.4
1	A	370	ARG	12.4
1	A	237	LEU	12.3
1	A	291	MET	11.8
1	A	371	LEU	11.7
1	A	263	LEU	11.6
1	A	211	GLU	11.5
1	A	246	ILE	11.4
1	A	221	GLN	11.3
1	A	316	GLY	11.1
1	A	353	ASN	11.1
1	A	210	ALA	11.0

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Mol	Chain	Res	Type	RSRZ
1	A	34	PRO	11.0
1	A	293	PHE	11.0
1	A	264	ASN	10.8
1	A	285	GLY	10.7
1	A	482	THR	10.6
1	A	209	PRO	10.6
1	A	231	VAL	10.5
1	A	214	ARG	10.5
1	A	228	SER	10.5
1	A	273	ALA	10.4
1	A	276	TYR	10.4
1	A	287	HIS	10.3
1	A	259	LYS	10.2
2	B	9	HIS	10.2
1	A	266	ASP	10.1
1	A	202	PRO	10.1
1	A	236	PHE	10.1
1	A	433	GLN	10.0
1	A	296	VAL	10.0
1	A	271	GLN	10.0
1	A	286	LYS	9.9
1	A	226	ALA	9.8
1	A	274	GLY	9.7
1	A	277	SER	9.7
1	A	216	ARG	9.7
1	A	351	LEU	9.6
1	A	289	THR	9.5
1	A	372	LYS	9.5
1	A	241	ASN	9.5
1	A	215	ILE	9.4
1	A	233	PHE	9.3
1	A	262	THR	9.1
1	A	261	LEU	9.1
1	A	298	SER	9.0
1	A	288	SER	9.0
1	A	282	ASN	9.0
1	A	498	PHE	9.0
1	A	294	ARG	8.9
2	B	29	THR	8.9
1	A	284	GLN	8.9
1	A	232	ASN	8.9
2	B	10	MET	8.8

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Mol	Chain	Res	Type	RSRZ
1	A	234	ASP	8.7
1	A	275	ASN	8.7
1	A	248	GLN	8.7
2	B	107	TYR	8.7
1	A	205	LEU	8.6
1	A	213	VAL	8.6
1	A	270	PHE	8.6
1	A	207	LEU	8.5
1	A	367	SER	8.5
1	A	369	PRO	8.4
1	A	281	SER	8.2
1	A	227	SER	8.2
1	A	212	LEU	8.2
2	B	26	GLN	8.2
1	A	208	VAL	8.1
1	A	201	GLY	8.1
1	A	350	LYS	8.0
1	A	315	VAL	8.0
1	A	74	ALA	7.9
1	A	317	GLU	7.9
1	A	199	ILE	7.9
1	A	280	ALA	7.9
1	A	240	ASN	7.8
1	A	375	GLU	7.7
1	A	96	ALA	7.6
1	A	224	CYS	7.4
1	A	239	HIS	7.4
1	A	398	LEU	7.4
1	A	73	ASN	7.3
1	A	238	GLN	7.3
1	A	279	VAL	7.3
1	A	314	THR	7.3
1	A	278	CYS	7.2
1	A	352	ALA	7.1
1	A	364	PHE	7.1
1	A	242	THR	7.0
1	A	33	LYS	7.0
1	A	36	ALA	7.0
2	B	27	MET	7.0
1	A	219	ALA	7.0
1	A	497	ALA	7.0
1	A	483	TYR	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	365	THR	7.0
1	A	366	LEU	7.0
2	B	7	CYS	7.0
1	A	95	ALA	6.9
1	A	318	GLY	6.9
2	B	30	SER	6.8
1	A	292	PHE	6.8
1	A	225	SER	6.8
1	A	360	TYR	6.7
2	B	108	GLU	6.7
1	A	122	ASP	6.7
1	A	368	LEU	6.7
1	A	347	PRO	6.6
2	B	102	CYS	6.6
2	B	35	PHE	6.6
1	A	75	THR	6.6
1	A	37	THR	6.5
1	A	206	THR	6.5
1	A	20	ILE	6.4
1	A	250	SER	6.3
1	A	94	SER	6.3
2	B	6	TYR	6.3
1	A	299	ALA	6.2
1	A	348	GLU	6.2
1	A	308	ASN	6.2
1	A	183	GLY	6.2
1	A	247	PRO	6.1
1	A	260	VAL	6.0
1	A	417	LEU	6.0
1	A	493	SER	6.0
2	B	86	ARG	6.0
2	B	33	ILE	6.0
1	A	373	PRO	5.9
2	B	4	SER	5.9
2	B	32	GLN	5.9
1	A	313	VAL	5.9
2	B	103	VAL	5.8
1	A	421	ALA	5.8
2	B	31	CYS	5.8
1	A	21	PRO	5.8
1	A	323	VAL	5.8
1	A	35	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	415	GLY	5.7
1	A	72	ASN	5.7
1	A	494	GLY	5.7
2	B	11	ILE	5.7
1	A	397	THR	5.7
1	A	300	TYR	5.7
1	A	448	GLN	5.6
1	A	328	TYR	5.5
1	A	336	TRP	5.5
1	A	283	VAL	5.5
2	B	101	ALA	5.5
1	A	229	VAL	5.5
1	A	307	GLN	5.4
1	A	223	VAL	5.3
1	A	200	PRO	5.3
1	A	320	ASN	5.2
1	A	197	LYS	5.2
1	A	102	LYS	5.1
2	B	25	SER	5.1
1	A	471	LEU	5.0
1	A	123	ALA	5.0
1	A	311	GLN	5.0
1	A	354	ALA	5.0
2	B	67	PHE	5.0
1	A	159	TRP	5.0
2	B	100	LYS	5.0
1	A	319	LEU	4.9
1	A	321	LEU	4.9
1	A	39	THR	4.9
2	B	5	GLU	4.9
1	A	38	VAL	4.9
1	A	49	GLU	4.9
1	A	450	TRP	4.9
1	A	257	TYR	4.9
1	A	429	VAL	4.8
2	B	42	GLN	4.8
1	A	245	ALA	4.8
2	B	15	HIS	4.8
1	A	396	LEU	4.8
1	A	23	ILE	4.8
1	A	158	PRO	4.8
1	A	258	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	4.7
1	A	32	VAL	4.7
2	B	8	SER	4.7
1	A	48	VAL	4.7
1	A	399	ARG	4.7
1	A	249	GLN	4.6
1	A	45	ASN	4.6
1	A	430	THR	4.6
1	A	451	ASP	4.6
1	A	447	LEU	4.6
2	B	2	GLU	4.6
2	B	34	THR	4.5
1	A	363	THR	4.5
1	A	428	ASN	4.5
1	A	470	SER	4.5
1	A	452	ASP	4.5
1	A	47	SER	4.4
1	A	46	GLY	4.4
1	A	329	PRO	4.4
1	A	379	TYR	4.4
2	B	3	VAL	4.4
1	A	243	LYS	4.4
1	A	395	GLU	4.4
1	A	495	SER	4.4
2	B	73	ASN	4.3
1	A	325	VAL	4.3
1	A	322	LYS	4.3
1	A	359	THR	4.3
2	B	28	GLU	4.3
1	A	492	GLY	4.2
1	A	44	GLY	4.2
2	B	106	PHE	4.2
1	A	59	THR	4.2
2	B	24	ASP	4.2
1	A	97	ILE	4.2
1	A	50	TRP	4.1
1	A	487	ALA	4.1
1	A	25	PRO	4.1
1	A	251	ASP	4.1
1	A	84	CYS	4.1
1	A	496	TRP	4.1
1	A	416	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	432	LEU	4.1
1	A	22	VAL	4.0
1	A	29	GLU	4.0
1	A	422	SER	4.0
1	A	400	TYR	4.0
1	A	408	TRP	4.0
1	A	312	GLU	4.0
1	A	193	LEU	3.9
1	A	431	TRP	3.9
2	B	68	ARG	3.9
1	A	355	THR	3.9
1	A	449	VAL	3.9
1	A	252	PHE	3.9
1	A	306	GLU	3.9
2	B	65	MET	3.8
1	A	42	CYS	3.8
1	A	362	HIS	3.8
1	A	255	ASN	3.8
1	A	28	PRO	3.8
1	A	374	SER	3.8
1	A	361	ARG	3.8
2	B	36	GLU	3.7
2	B	110	PRO	3.7
1	A	484	GLU	3.6
1	A	43	VAL	3.6
1	A	346	GLN	3.6
1	A	164	ILE	3.6
1	A	91	LEU	3.6
1	A	327	ALA	3.6
1	A	305	SER	3.6
1	A	103	ASP	3.5
1	A	81	THR	3.5
1	A	486	ARG	3.5
1	A	337	THR	3.5
1	A	71	THR	3.5
1	A	31	VAL	3.4
1	A	93	GLY	3.4
1	A	182	GLY	3.4
1	A	26	SER	3.4
1	A	381	PHE	3.4
1	A	309	LEU	3.4
2	B	105	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	401	PRO	3.3
1	A	488	HIS	3.3
1	A	56	PRO	3.3
2	B	70	ASN	3.3
1	A	92	GLY	3.3
2	B	64	THR	3.3
1	A	67	SER	3.3
1	A	331	LEU	3.2
1	A	57	HIS	3.2
1	A	403	GLU	3.2
2	B	37	PHE	3.2
1	A	326	GLU	3.1
1	A	85	THR	3.1
2	B	12	GLY	3.0
1	A	330	GLY	3.0
1	A	175	TYR	3.0
2	B	114	LEU	3.0
1	A	345	HIS	3.0
1	A	146	ARG	3.0
1	A	107	PRO	3.0
1	A	324	MET	3.0
1	A	101	VAL	3.0
2	B	117	VAL	3.0
1	A	376	ALA	2.9
1	A	410	PHE	2.9
1	A	393	THR	2.9
1	A	70	SER	2.9
2	B	23	ILE	2.9
1	A	469	GLN	2.9
2	B	95	TYR	2.9
1	A	394	PHE	2.8
1	A	130	THR	2.8
1	A	98	HIS	2.8
1	A	132	PRO	2.8
1	A	82	TYR	2.8
1	A	61	TYR	2.7
1	A	129	LEU	2.7
1	A	468	VAL	2.7
1	A	173	GLN	2.7
1	A	41	ARG	2.7
1	A	485	CYS	2.7
1	A	117	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	124	THR	2.7
1	A	121	GLN	2.7
1	A	27	VAL	2.6
1	A	420	ALA	2.6
2	B	22	LEU	2.6
1	A	142	ARG	2.6
2	B	141	ASN	2.6
1	A	135	GLU	2.6
2	B	79	GLN	2.6
1	A	198	VAL	2.5
1	A	140	LEU	2.5
2	B	83	LEU	2.5
1	A	54	PRO	2.5
1	A	339	LEU	2.5
2	B	87	LEU	2.5
2	B	41	GLU	2.5
1	A	334	PHE	2.5
2	B	69	ASP	2.5
1	A	100	TYR	2.5
1	A	40	LEU	2.5
2	B	16	LEU	2.4
2	B	104	ARG	2.4
2	B	71	THR	2.4
1	A	66	SER	2.4
1	A	406	VAL	2.4
1	A	386	PRO	2.4
1	A	387	GLY	2.4
1	A	68	ILE	2.4
1	A	302	ASN	2.4
2	B	116	LYS	2.4
1	A	78	ASN	2.4
1	A	491	VAL	2.4
1	A	385	ASN	2.4
1	A	303	LEU	2.3
2	B	146	CYS	2.3
1	A	60	LEU	2.3
1	A	83	ARG	2.3
1	A	184	ARG	2.3
1	A	172	SER	2.3
1	A	253	HIS	2.3
2	B	113	LEU	2.3
1	A	407	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	455	PRO	2.3
2	B	109	THR	2.2
2	B	94	ASP	2.2
2	B	72	PRO	2.2
2	B	38	VAL	2.2
2	B	76	ALA	2.2
1	A	147	PRO	2.2
2	B	84	SER	2.1
1	A	113	GLN	2.1
2	B	62	GLU	2.1
1	A	404	VAL	2.1
2	B	121	PHE	2.1
1	A	465	LYS	2.1
1	A	156	PHE	2.0
2	B	111	LEU	2.0
1	A	310	ILE	2.0
1	A	131	ASP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.