



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:58 AM UTC

PDB ID : 4WRM / pdb_00004wrn
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

<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
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

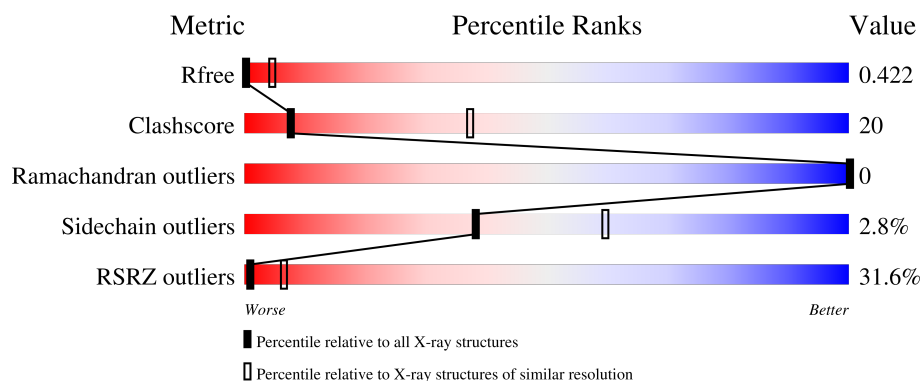
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1166 (9.70-4.00)
Clashscore	190562	1006 (9.50-4.04)
Ramachandran outliers	187476	1053 (9.70-4.00)
Sidechain outliers	187428	1016 (9.70-4.00)
RSRZ outliers	180081	1159 (9.70-4.00)

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	493	28% 65% 22% 10%
2	B	170	28% 73% 10% 17%

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:

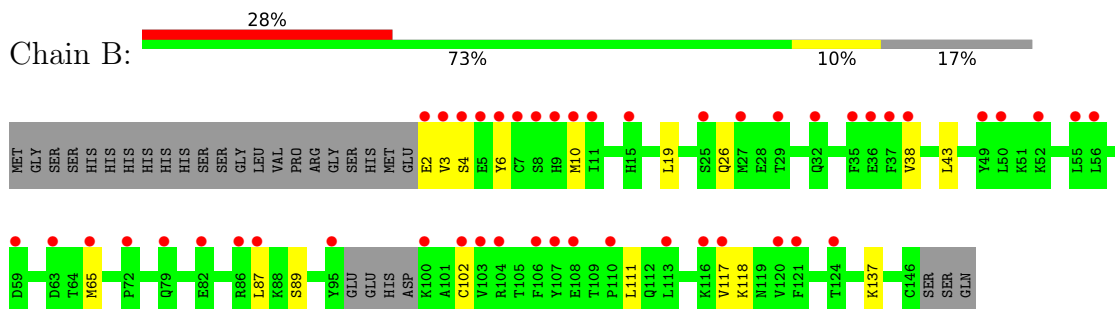
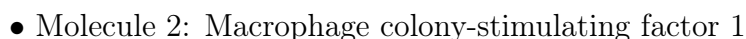
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP P09603
B	-19	GLY	-	expression tag	UNP P09603
B	-18	SER	-	expression tag	UNP P09603
B	-17	SER	-	expression tag	UNP P09603
B	-16	HIS	-	expression tag	UNP P09603
B	-15	HIS	-	expression tag	UNP P09603
B	-14	HIS	-	expression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

- Molecule 1: Macrophage colony-stimulating factor 1 receptor



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 – 6.85	Depositor EDS
% Data completeness (in resolution range)	82.7 (48.75-6.85) 99.5 (48.75-6.85)	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 0.355 , 0.422	Depositor DCC
R_{free} test set	396 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	446.7	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 756.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	1/3509 (0.0%)	1.02	18/4788 (0.4%)
2	B	0.33	0/1118	0.70	0/1513
All	All	0.57	1/4627 (0.0%)	0.95	18/6301 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	ASN	CA-C	5.15	1.59	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	GLN	CA-C-N	9.79	130.21	120.52
1	A	426	GLN	C-N-CA	9.79	130.21	120.52
1	A	452	ASP	CA-C-N	7.57	129.30	119.84
1	A	452	ASP	C-N-CA	7.57	129.30	119.84
1	A	463	PHE	N-CA-C	7.49	121.85	111.74
1	A	454	TYR	CA-C-N	7.04	128.64	119.84
1	A	454	TYR	C-N-CA	7.04	128.64	119.84
1	A	461	GLU	N-CA-C	6.93	118.52	109.93
1	A	424	TYR	N-CA-C	-6.55	101.03	110.40
1	A	491	VAL	N-CA-C	6.07	117.62	111.00
1	A	91	LEU	N-CA-C	-6.02	105.89	113.23
1	A	407	ILE	N-CA-C	5.89	116.96	108.48
1	A	448	GLN	N-CA-C	5.76	117.61	108.79
1	A	404	VAL	N-CA-C	5.66	116.10	108.17
1	A	458	LEU	N-CA-C	5.46	119.90	112.04
1	A	240	ASN	CB-CA-C	-5.20	110.16	117.23
1	A	406	VAL	N-CA-C	5.08	115.17	107.80
1	A	457	VAL	N-CA-C	5.07	116.04	108.54

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	3422	0	3286	165	4
2	B	1102	0	1034	14	0
All	All	4524	0	4320	178	4

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 (178) 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
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:CG2	1:A:298:SER:C	2.16	1.18
1:A:215:ILE:HD13	1:A:299:ALA:CA	1.65	1.17
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PRO:C	1:A:106:ARG:HG2	1.83	1.03
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:215:ILE:HG23	1:A:298:SER:C	1.81	0.99
1:A:28:PRO:C	1:A:159:TRP:HZ2	1.72	0.97
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: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:215:ILE:HG21	1:A:298:SER:C	1.88	0.90
1:A:338:TYR:CE2	1:A:340:GLY:O	2.25	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:104:PRO:O	1:A:106:ARG:HG2	1.74	0.86
1:A:29:GLU:OE2	1:A:132:PRO:HG3	1.76	0.85
1:A:214:ARG:NH1	1:A:328:TYR:CZ	2.31	0.84
1:A:215:ILE:HD11	1:A:299:ALA:HA	0.86	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:100:TYR:CD1	1:A:130:THR:HA	2.15	0.81
1:A:342:PHE:CG	1:A:374:SER:HA	2.16	0.81
1:A:463:PHE:O	1:A:463:PHE:CD2	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:338:TYR:CZ	1:A:340:GLY:C	2.63	0.76
1:A:181:MET:HE2	1:A:186:VAL:HG11	1.66	0.76
1:A:214:ARG:NH1	1:A:328:TYR:CE1	2.55	0.74
1:A:215:ILE:CG1	1:A:298:SER:C	2.60	0.74
1:A:215:ILE:HD13	1:A:298:SER:C	2.13	0.73
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:463:PHE:O	1:A:463:PHE:CG	2.43	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HG12	1:A:298:SER:C	2.17	0.70
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: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:400:TYR:HB2	1:A:423:GLY:HA2	1.79	0.65
1:A:28:PRO:C	1:A:159:TRP:CZ2	2.54	0.64
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:89:ASP:OD1	1:A:90:PRO:HD2	1.98	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:430:THR:HB	1:A:486:ARG:HB2	1.79	0.63
1:A:104:PRO:C	1:A:105:ALA:HB3	2.16	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
1:A:338:TYR:CE2	1:A:340:GLY:C	2.78	0.60
1:A:240:ASN:OD1	1:A:240:ASN:N	2.33	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:215:ILE:CD1	1:A:298:SER:C	2.72	0.60
1:A:98:HIS:CE1	1:A:159:TRP:O	2.54	0.59
1:A:215:ILE:HD11	1:A:299:ALA:CB	2.31	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: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:104:PRO:C	1:A:106:ARG:CG	2.71	0.57
1:A:324:MET:HG3	1:A:363:THR:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:459:SER:HB2	1:A:467:THR:OG1	2.05	0.56
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:421:ALA:O	1:A:468:VAL:HG22	2.08	0.53
1:A:432:LEU:O	1:A:484:GLU:HB3	2.07	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:35:GLY:HA2	1:A:73:ASN:OD1	2.10	0.52
1:A:215:ILE:CD1	1:A:299:ALA:HB2	2.39	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
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
1:A:431:TRP:CZ3	1:A:485:CYS:HB2	2.49	0.47
2:B:3:VAL:CG2	2:B:89:SER:O	2.56	0.47
1:A:103:ASP:O	1:A:106:ARG:CB	2.53	0.47
1:A:239:HIS:C	1:A:240:ASN:OD1	2.58	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: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:400:TYR:CD2	1:A:465:LYS:HD3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:65:MET:HE1	2:B:117:VAL:HG21	2.00	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
2:B:10:MET:HE3	2:B:87:LEU:HD23	2.00	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: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:404:VAL:HG13	1:A:419:CYS:SG	2.59	0.42
1:A:215:ILE:CB	1:A:298:SER:C	2.90	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:53:PRO:HA	1:A:54:PRO:HD3	1.97	0.41
1:A:402:PRO:HA	1:A:422:SER:O	2.20	0.41
1:A:231:VAL:HG11	2:B:10:MET:SD	2.61	0.41
1:A:146:ARG:H	1:A:146:ARG:HG2	1.62	0.41
1:A:406:VAL:HA	1:A:418:LEU:O	2.21	0.41
2:B:2:GLU:O	2:B:2:GLU:HG2	2.20	0.41
2:B:38:VAL:HG23	2:B:43:LEU:HD13	2.02	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 (4) 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:60:LEU:O	1:A:61:TYR:CD1[10_665]	1.31	0.89
1:A:370:ARG:NH2	1:A:375:GLU:OE2[9_554]	1.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:CD2	1:A:452:ASP:OD1[12_565]	2.11	0.09
1:A:370:ARG:NH1	1:A:375:GLU:OE1[9_554]	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 [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	372/429 (87%)	358 (96%)	14 (4%)	29	50
2	B	122/160 (76%)	122 (100%)	0	100	100
All	All	494/589 (84%)	480 (97%)	14 (3%)	38	60

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ARG

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Mol	Chain	Res	Type
1	A	186	VAL
1	A	198	VAL
1	A	240	ASN
1	A	279	VAL
1	A	313	VAL
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	458	LEU
1	A	461	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	113	GLN
1	A	238	GLN
1	A	248	GLN
1	A	345	HIS
1	A	433	GLN
1	A	464	HIS
2	B	42	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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%)	1.62	138 (31%)  	216, 314, 410, 458	0
2	B	141/170 (82%)	1.70	47 (33%)  	213, 290, 416, 477	0
All	All	586/663 (88%)	1.64	185 (31%)  	213, 307, 411, 477	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	VAL	16.8
1	A	204	ALA	16.3
1	A	105	ALA	13.1
2	B	10	MET	11.5
1	A	231	VAL	11.3
1	A	294	ARG	11.1
2	B	4	SER	10.6
1	A	232	ASN	9.9
2	B	6	TYR	9.7
1	A	220	ALA	8.6
1	A	283	VAL	8.6
1	A	265	LEU	7.9
1	A	234	ASP	7.9
1	A	135	GLU	7.7
2	B	107	TYR	7.1
1	A	236	PHE	7.1
1	A	373	PRO	7.1
1	A	292	PHE	6.3
1	A	230	ASP	6.3
1	A	104	PRO	6.2
1	A	72	ASN	6.0
1	A	203	PRO	6.0
1	A	39	THR	5.9
1	A	293	PHE	5.9

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Mol	Chain	Res	Type	RSRZ
2	B	9	HIS	5.8
2	B	108	GLU	5.7
2	B	11	ILE	5.7
1	A	273	ALA	5.6
2	B	5	GLU	5.4
1	A	286	LYS	5.3
1	A	471	LEU	5.2
1	A	463	PHE	5.0
1	A	226	ALA	5.0
1	A	235	VAL	4.9
1	A	228	SER	4.9
1	A	229	VAL	4.9
1	A	70	SER	4.8
1	A	59	THR	4.8
2	B	106	PHE	4.6
1	A	33	LYS	4.6
2	B	79	GLN	4.5
1	A	62	SER	4.5
1	A	259	LYS	4.4
1	A	182	GLY	4.4
1	A	281	SER	4.4
1	A	61	TYR	4.4
1	A	498	PHE	4.4
1	A	334	PHE	4.4
1	A	91	LEU	4.3
2	B	121	PHE	4.3
2	B	124	THR	4.3
1	A	415	GLY	4.3
2	B	35	PHE	4.3
1	A	107	PRO	4.3
2	B	52	LYS	4.2
1	A	285	GLY	4.1
1	A	284	GLN	4.1
1	A	211	GLU	4.1
1	A	102	LYS	4.0
1	A	103	ASP	3.9
1	A	397	THR	3.9
2	B	95	TYR	3.9
1	A	282	ASN	3.9
2	B	103	VAL	3.9
1	A	227	SER	3.7
2	B	50	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	243	LYS	3.6
1	A	159	TRP	3.6
2	B	32	GLN	3.6
1	A	93	GLY	3.5
1	A	272	HIS	3.5
2	B	8	SER	3.4
1	A	375	GLU	3.4
1	A	352	ALA	3.3
1	A	233	PHE	3.3
2	B	72	PRO	3.3
1	A	395	GLU	3.3
1	A	205	LEU	3.3
2	B	55	LEU	3.3
2	B	120	VAL	3.2
1	A	426	GLN	3.2
2	B	104	ARG	3.2
2	B	100	LYS	3.2
1	A	416	THR	3.1
2	B	7	CYS	3.1
1	A	60	LEU	3.1
1	A	183	GLY	3.1
1	A	73	ASN	3.1
1	A	275	ASN	3.1
1	A	37	THR	3.1
1	A	20	ILE	3.0
1	A	34	PRO	3.0
2	B	3	VAL	3.0
1	A	158	PRO	3.0
1	A	274	GLY	3.0
2	B	27	MET	3.0
1	A	381	PHE	3.0
2	B	37	PHE	3.0
1	A	206	THR	2.9
1	A	208	VAL	2.9
1	A	47	SER	2.9
1	A	255	ASN	2.9
1	A	25	PRO	2.9
1	A	248	GLN	2.9
1	A	214	ARG	2.9
2	B	49	TYR	2.9
1	A	337	THR	2.9
1	A	109	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	266	ASP	2.8
2	B	102	CYS	2.8
2	B	113	LEU	2.8
1	A	345	HIS	2.7
1	A	94	SER	2.7
1	A	264	ASN	2.7
2	B	29	THR	2.7
1	A	464	HIS	2.7
1	A	209	PRO	2.7
1	A	173	GLN	2.7
1	A	495	SER	2.7
1	A	90	PRO	2.7
1	A	172	SER	2.6
1	A	424	TYR	2.6
1	A	455	PRO	2.6
2	B	36	GLU	2.6
1	A	225	SER	2.6
1	A	200	PRO	2.6
1	A	401	PRO	2.6
1	A	106	ARG	2.6
1	A	466	VAL	2.6
1	A	132	PRO	2.6
1	A	262	THR	2.6
1	A	279	VAL	2.6
2	B	63	ASP	2.5
1	A	26	SER	2.5
1	A	92	GLY	2.5
1	A	24	GLU	2.5
1	A	181	MET	2.5
1	A	210	ALA	2.5
1	A	111	LEU	2.4
1	A	465	LYS	2.4
2	B	110	PRO	2.4
1	A	410	PHE	2.4
1	A	343	SER	2.4
1	A	46	GLY	2.4
1	A	28	PRO	2.4
1	A	462	PRO	2.4
1	A	447	LEU	2.4
2	B	56	LEU	2.4
1	A	378	ARG	2.4
1	A	417	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	403	GLU	2.3
2	B	38	VAL	2.3
1	A	213	VAL	2.3
2	B	82	GLU	2.3
1	A	269	ASP	2.3
1	A	276	TYR	2.3
1	A	35	GLY	2.3
2	B	117	VAL	2.2
1	A	108	TRP	2.2
1	A	490	SER	2.2
1	A	467	THR	2.2
2	B	2	GLU	2.2
1	A	353	ASN	2.2
1	A	116	VAL	2.2
1	A	460	GLN	2.2
1	A	312	GLU	2.2
2	B	59	ASP	2.1
1	A	386	PRO	2.1
2	B	15	HIS	2.1
2	B	25	SER	2.1
2	B	116	LYS	2.1
1	A	383	ALA	2.1
2	B	65	MET	2.1
2	B	87	LEU	2.1
1	A	190	SER	2.1
1	A	369	PRO	2.1
1	A	151	HIS	2.1
1	A	68	ILE	2.1
1	A	221	GLN	2.1
1	A	469	GLN	2.1
2	B	86	ARG	2.0
1	A	391	ALA	2.0
1	A	31	VAL	2.0
1	A	408	TRP	2.0
1	A	332	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.