



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 12:45 PM JST

PDB ID : 9UVE / pdb_00009uve
Title : Crystal structure of Sec23a/24a/22b bound to STING FpS motif
Authors : Ma, W.F.
Deposited on : 2025-05-10
Resolution : 2.60 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 : 1.8.5 (274361), CSD as541be (2020)
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

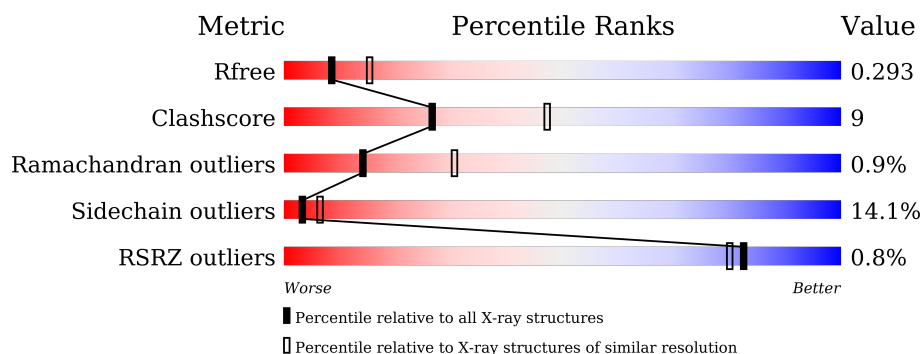
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	765	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 68% 22% • 7% </div> </div>
2	B	747	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 62% 31% • • </div> </div>
3	C	157	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 61% 20% • • 17% </div> </div>
4	D	2	<div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 50% 50% </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12479 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	0	0
			5609	3577	960	1032	40			

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	732	Total	C	N	O	S	0	0	0
			5715	3649	963	1069	34			

- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	131	Total	C	N	O	S	0	0	0
			1044	674	166	196	8			

- Molecule 4 is a protein called PHE-SEP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	P	0	0	0
			22	12	2	7	1			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

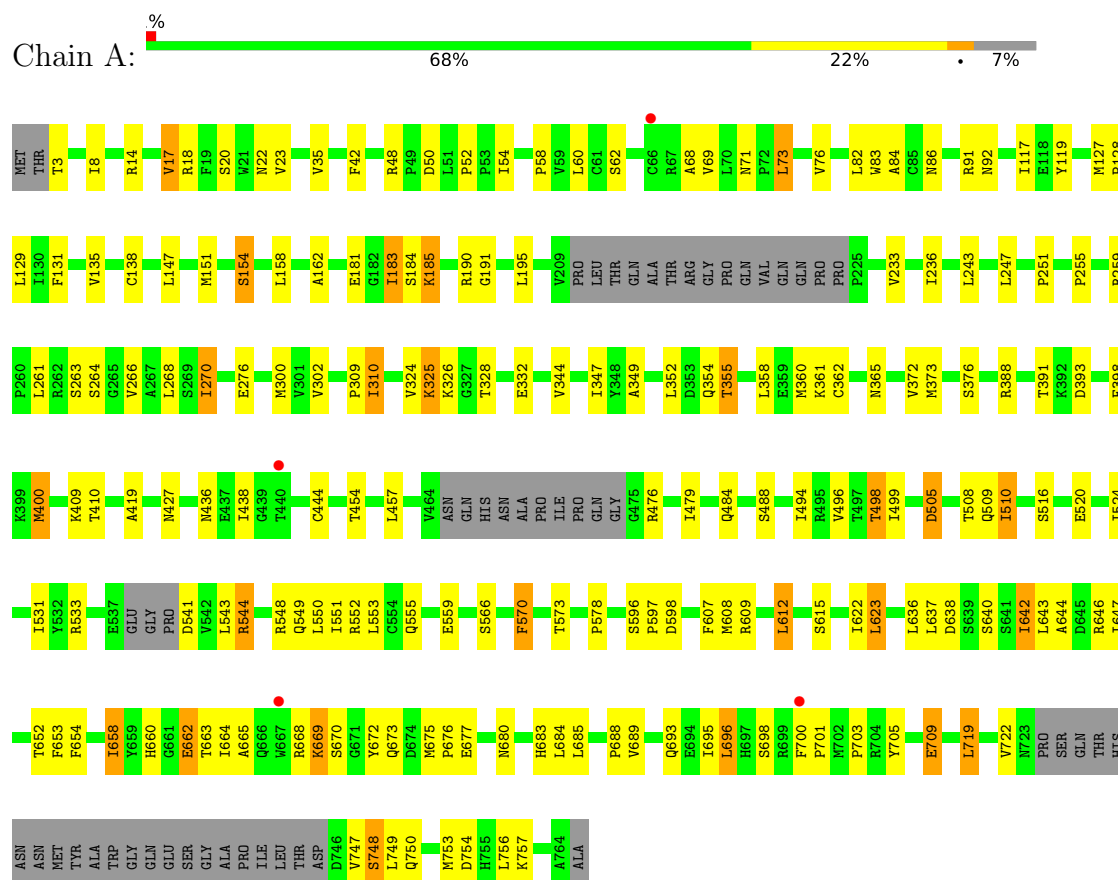
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total 41	O 41	0	0
6	B	43	Total 43	O 43	0	0
6	C	3	Total 3	O 3	0	0

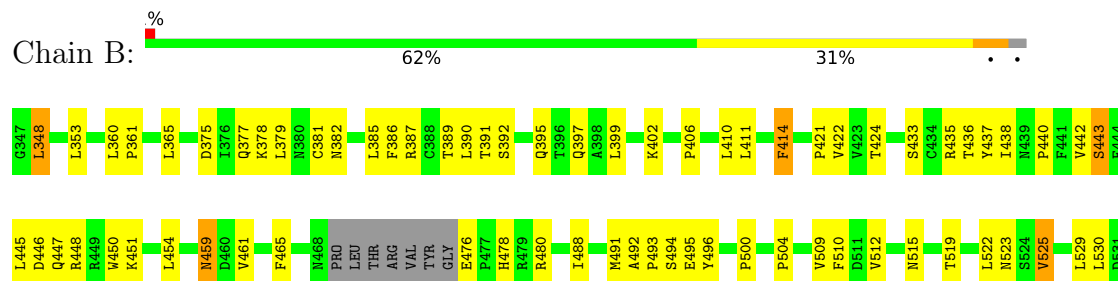
3 Residue-property plots [i](#)

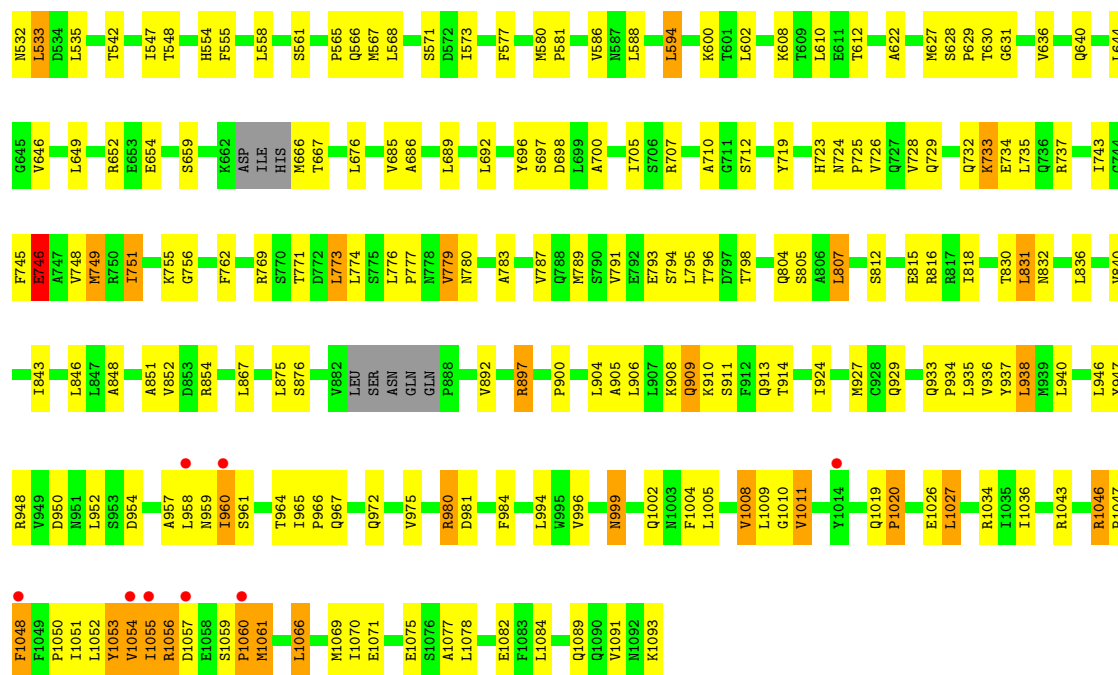
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein transport protein Sec23A

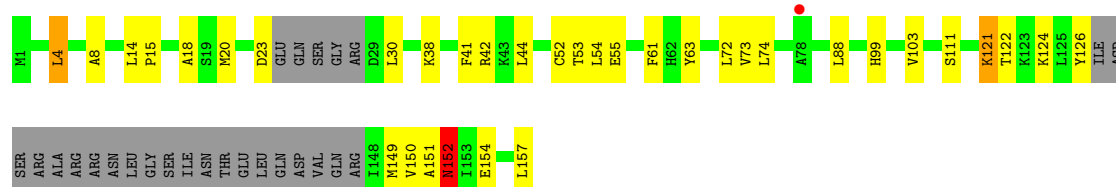


• Molecule 2: Protein transport protein Sec24A





• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: PHE-SEP



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.26Å 98.17Å 130.12Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	19.88 – 2.60 19.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.88-2.60) 97.3 (19.88-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.59Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.233 , 0.291 0.239 , 0.293	Depositor DCC
R_{free} test set	1997 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12479	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/5740	0.63	0/7777
2	B	0.34	0/5837	0.57	2/7943 (0.0%)
3	C	0.38	0/1063	0.61	0/1434
4	D	0.10	0/11	0.20	0/13
All	All	0.37	0/12651	0.60	2/17167 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1053	TYR	CB-CA-C	5.93	122.23	110.42
2	B	1053	TYR	CA-CB-CG	5.47	123.75	113.90

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	5609	0	5519	91	0
2	B	5715	0	5711	122	0
3	C	1044	0	1036	21	0
4	D	22	0	14	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	41	0	0	2	0
6	B	43	0	0	1	0
6	C	3	0	0	0	0
All	All	12479	0	12280	230	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 9.

All (230) 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)
3:C:15:PRO:HG3	3:C:38:LYS:HZ1	1.39	0.86
2:B:980:ARG:H	2:B:980:ARG:HE	1.26	0.82
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.62	0.81
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.64	0.80
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.68	0.76
1:A:127:MET:HG3	1:A:128:PRO:HD2	1.69	0.73
3:C:73:VAL:HB	3:C:88:LEU:HD21	1.71	0.72
2:B:1043:ARG:HG2	2:B:1050:PRO:HD2	1.70	0.72
2:B:438:ILE:HG13	2:B:442:VAL:HG21	1.72	0.72
2:B:510:PHE:HB2	2:B:548:THR:HG22	1.73	0.69
2:B:960:ILE:HG13	2:B:965:ILE:HD13	1.74	0.69
1:A:259:ARG:HH22	1:A:309:PRO:HA	1.58	0.69
2:B:756:GLY:HA2	2:B:793:GLU:HB2	1.75	0.69
1:A:644:ALA:HB1	1:A:663:THR:HG22	1.75	0.68
2:B:958:LEU:HA	2:B:964:THR:HA	1.75	0.68
2:B:530:LEU:HD11	2:B:600:LYS:HE3	1.75	0.67
2:B:1046:ARG:HD2	2:B:1050:PRO:HG3	1.77	0.67
1:A:623:LEU:HD12	1:A:637:LEU:HD23	1.78	0.66
1:A:347:ILE:HD13	1:A:360:MET:HE3	1.77	0.65
1:A:484:GLN:HB3	1:A:494:ILE:HG12	1.78	0.65
2:B:958:LEU:HB3	2:B:964:THR:HG22	1.79	0.65
1:A:658:ILE:HG13	1:A:705:TYR:HE1	1.63	0.64
1:A:643:LEU:HB2	1:A:646:ARG:HG3	1.79	0.64
2:B:1026:GLU:HG2	2:B:1036:ILE:HD13	1.79	0.64
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.81	0.63
2:B:776:LEU:HD23	2:B:779:VAL:HB	1.82	0.62
3:C:14:LEU:HD12	3:C:15:PRO:HD2	1.82	0.61
1:A:195:LEU:HD12	1:A:270:ILE:HD11	1.82	0.60
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:THR:HG22	1:A:479:ILE:HG12	1.84	0.60
1:A:68:ALA:HA	1:A:409:LYS:HE3	1.82	0.59
2:B:924:ILE:HD13	2:B:927:MET:HE2	1.85	0.59
2:B:443:SER:HB2	2:B:451:LYS:HB3	1.86	0.58
2:B:558:LEU:HD12	2:B:594:LEU:HG	1.84	0.58
1:A:660:HIS:HB2	1:A:709:GLU:HB3	1.85	0.58
2:B:840:VAL:HG12	6:B:1215:HOH:O	2.02	0.58
3:C:54:LEU:HB2	3:C:61:PHE:HB2	1.85	0.57
2:B:530:LEU:HA	2:B:533:LEU:HD22	1.87	0.57
2:B:1066:LEU:HA	2:B:1069:MET:HG2	1.87	0.57
1:A:8:ILE:HD11	1:A:22:ASN:HD21	1.70	0.57
2:B:436:THR:HG21	2:B:454:LEU:HD13	1.86	0.56
2:B:908:LYS:HE2	2:B:1077:ALA:HB1	1.87	0.56
2:B:1005:LEU:HD12	2:B:1011:VAL:HG23	1.88	0.56
1:A:541:ASP:HB3	1:A:544:ARG:HG3	1.87	0.56
1:A:135:VAL:HG22	1:A:151:MET:HE1	1.87	0.56
2:B:532:ASN:HB2	2:B:535:LEU:HB2	1.88	0.55
2:B:1054:VAL:O	2:B:1055:ILE:C	2.49	0.55
2:B:729:GLN:O	2:B:733:LYS:HG2	2.06	0.55
2:B:446:ASP:C	2:B:448:ARG:H	2.15	0.55
2:B:909:GLN:HG2	2:B:910:LYS:N	2.22	0.54
1:A:660:HIS:HB3	1:A:664:ILE:HG22	1.89	0.54
2:B:442:VAL:HG11	2:B:450:TRP:HB2	1.89	0.54
1:A:647:ILE:HG12	1:A:664:ILE:HG21	1.90	0.54
1:A:638:ASP:C	1:A:640:SER:H	2.16	0.54
2:B:686:ALA:HB2	2:B:777:PRO:HB2	1.90	0.54
1:A:69:VAL:HG11	1:A:496:VAL:HG21	1.91	0.53
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.91	0.53
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.91	0.53
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.91	0.53
1:A:147:LEU:HD11	1:A:151:MET:HE3	1.90	0.53
2:B:948:ARG:HB3	2:B:984:PHE:CE2	2.44	0.53
2:B:652:ARG:HD3	2:B:696:TYR:OH	2.09	0.53
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.91	0.53
1:A:670:SER:C	1:A:672:TYR:H	2.17	0.53
2:B:749:MET:HG3	2:B:807:LEU:HD13	1.91	0.52
1:A:524:ILE:HD12	1:A:615:SER:HB3	1.91	0.52
3:C:121:LYS:HD3	3:C:122:THR:HG23	1.92	0.52
2:B:555:PHE:HZ	2:B:622:ALA:HB1	1.73	0.52
3:C:38:LYS:HA	3:C:41:PHE:HD2	1.74	0.52
2:B:975:VAL:HA	2:B:1069:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:GLU:HB2	2:B:478:HIS:CE1	2.45	0.51
3:C:99:HIS:O	3:C:103:VAL:HG23	2.10	0.51
3:C:55:GLU:H	3:C:151:ALA:HB1	1.76	0.51
2:B:1057:ASP:N	2:B:1060:PRO:HG3	2.24	0.50
2:B:399:LEU:HD11	2:B:831:LEU:HA	1.92	0.50
2:B:952:LEU:HD13	2:B:966:PRO:HG2	1.94	0.50
1:A:354:GLN:NE2	1:A:598:ASP:H	2.10	0.50
1:A:549:GLN:HE22	1:A:552:ARG:HH11	1.58	0.50
2:B:493:PRO:HD2	2:B:496:TYR:CD2	2.45	0.50
2:B:360:LEU:HD12	2:B:361:PRO:HD2	1.93	0.50
1:A:35:VAL:HG11	1:A:553:LEU:HB2	1.94	0.49
1:A:696:LEU:HD12	1:A:703:PRO:HD2	1.93	0.49
2:B:848:ALA:HB2	2:B:906:LEU:HD21	1.95	0.49
2:B:379:LEU:HD13	2:B:440:PRO:HB3	1.94	0.49
2:B:1019:GLN:HG3	2:B:1061:MET:HE1	1.93	0.49
2:B:353:LEU:HD13	2:B:900:PRO:HG3	1.95	0.49
2:B:395:GLN:NE2	2:B:796:THR:HA	2.27	0.49
3:C:154:GLU:HA	3:C:157:LEU:HD22	1.94	0.49
1:A:191:GLY:HA2	1:A:266:VAL:HG11	1.95	0.48
2:B:745:PHE:O	2:B:746:GLU:C	2.55	0.48
2:B:465:PHE:HA	2:B:480:ARG:HE	1.78	0.48
2:B:905:ALA:HB2	2:B:1070:ILE:HD13	1.95	0.48
1:A:693:GLN:HA	1:A:696:LEU:HB2	1.95	0.48
2:B:676:LEU:HD23	2:B:705:ILE:HD11	1.96	0.48
2:B:769:ARG:HB2	2:B:773:LEU:HD23	1.96	0.48
1:A:531:ILE:HG22	1:A:608:MET:HE2	1.95	0.47
3:C:20:MET:HB3	3:C:30:LEU:HD21	1.95	0.47
1:A:183:ILE:HD12	2:B:567:MET:HB2	1.96	0.47
2:B:631:GLY:HA2	2:B:685:VAL:CG2	2.44	0.47
1:A:162:ALA:O	1:A:233:VAL:HG23	2.15	0.47
1:A:652:THR:O	1:A:653:PHE:C	2.55	0.47
1:A:398:PHE:HB3	1:A:400:MET:HG3	1.97	0.47
2:B:421:PRO:HG2	2:B:488:ILE:HG13	1.96	0.47
2:B:780:ASN:HD21	2:B:783:ALA:HB2	1.79	0.47
1:A:373:MET:HE2	1:A:373:MET:HB3	1.80	0.47
2:B:832:ASN:O	2:B:836:LEU:HG	2.15	0.47
2:B:437:TYR:HB2	2:B:804:GLN:HE22	1.79	0.47
2:B:397:GLN:HB2	2:B:791:VAL:O	2.14	0.47
2:B:762:PHE:CD2	2:B:774:LEU:HD21	2.50	0.47
1:A:419:ALA:HB1	1:A:457:LEU:HD12	1.97	0.46
2:B:897:ARG:H	2:B:897:ARG:HG3	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:O	1:A:158:LEU:HG	2.15	0.46
2:B:390:LEU:C	2:B:392:SER:H	2.23	0.46
2:B:904:LEU:HD11	2:B:908:LYS:HE3	1.98	0.46
1:A:8:ILE:HD11	1:A:22:ASN:ND2	2.31	0.46
2:B:1004:PHE:CE1	2:B:1008:VAL:HG21	2.51	0.46
1:A:276:GLU:HB2	6:A:912:HOH:O	2.16	0.45
1:A:505:ASP:O	1:A:509:GLN:N	2.49	0.45
2:B:525:VAL:HG22	2:B:735:LEU:HD11	1.98	0.45
2:B:734:GLU:HA	2:B:1048:PHE:HE1	1.81	0.45
1:A:670:SER:C	1:A:672:TYR:N	2.74	0.45
1:A:647:ILE:HD11	1:A:685:LEU:HD23	1.99	0.45
2:B:504:PRO:HG2	2:B:542:THR:HA	1.97	0.45
1:A:520:GLU:O	1:A:524:ILE:HG12	2.16	0.45
1:A:14:ARG:HG3	1:A:48:ARG:HH22	1.81	0.45
1:A:14:ARG:HG3	1:A:48:ARG:NH2	2.31	0.45
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.98	0.45
2:B:737:ARG:NH1	2:B:1047:PRO:HB2	2.32	0.45
1:A:310:ILE:H	1:A:310:ILE:HG13	1.45	0.45
3:C:15:PRO:HG3	3:C:38:LYS:NZ	2.21	0.45
2:B:959:ASN:O	2:B:960:ILE:C	2.59	0.45
3:C:124:LYS:C	3:C:126:TYR:H	2.25	0.45
2:B:851:ALA:HB2	2:B:867:LEU:HD21	1.98	0.44
1:A:302:VAL:HB	1:A:310:ILE:HG23	1.99	0.44
1:A:325:LYS:HE2	1:A:325:LYS:HB3	1.41	0.44
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.52	0.44
2:B:935:LEU:HD12	2:B:938:LEU:HD12	1.98	0.44
1:A:251:PRO:HG2	2:B:580:MET:HE2	1.98	0.44
2:B:382:ASN:HB2	2:B:385:LEU:HD12	2.00	0.44
1:A:361:LYS:HB2	1:A:361:LYS:NZ	2.33	0.44
1:A:652:THR:C	1:A:654:PHE:N	2.75	0.44
2:B:509:VAL:HA	2:B:547:ILE:O	2.18	0.44
2:B:1066:LEU:HD23	2:B:1066:LEU:H	1.82	0.44
1:A:190:ARG:NH2	2:B:577:PHE:HB3	2.32	0.44
2:B:496:TYR:CD2	2:B:818:ILE:HD11	2.53	0.44
2:B:751:ILE:HG23	2:B:805:SER:HB3	1.99	0.44
1:A:84:ALA:HB2	1:A:91:ARG:HD3	2.00	0.44
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.33	0.44
2:B:515:ASN:O	2:B:519:THR:HG23	2.18	0.44
3:C:4:LEU:HD23	3:C:74:LEU:HD23	1.99	0.44
1:A:673:GLN:HG2	1:A:685:LEU:HD12	2.00	0.43
3:C:4:LEU:HD13	3:C:20:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.53	0.43
2:B:414:PHE:CD2	2:B:779:VAL:HG22	2.54	0.43
2:B:723:HIS:O	2:B:725:PRO:HD3	2.18	0.43
2:B:929:GLN:O	2:B:933:GLN:HB2	2.17	0.43
1:A:684:LEU:O	1:A:688:PRO:HD3	2.18	0.43
2:B:608:LYS:HB3	2:B:608:LYS:HE2	1.75	0.43
2:B:724:ASN:O	2:B:728:VAL:HG23	2.17	0.43
2:B:909:GLN:OE1	2:B:911:SER:HB2	2.19	0.43
2:B:934:PRO:HG2	2:B:937:TYR:HD2	1.83	0.43
2:B:1027:LEU:H	2:B:1027:LEU:HD12	1.83	0.43
2:B:381:CYS:SG	2:B:386:PHE:HB3	2.58	0.43
1:A:550:LEU:HD11	1:A:578:PRO:HB3	2.00	0.43
1:A:665:ALA:HB2	1:A:709:GLU:HB2	2.00	0.43
2:B:1055:ILE:O	2:B:1057:ASP:N	2.51	0.43
2:B:910:LYS:HA	2:B:913:GLN:CD	2.44	0.43
1:A:719:LEU:H	1:A:719:LEU:HG	1.55	0.43
1:A:754:ASP:HA	1:A:757:LYS:HB2	1.99	0.43
1:A:358:LEU:HD12	1:A:361:LYS:HE3	2.00	0.43
1:A:749:LEU:O	1:A:750:GLN:C	2.61	0.43
2:B:406:PRO:HB2	2:B:846:LEU:HD23	2.00	0.43
1:A:50:ASP:HA	6:A:913:HOH:O	2.19	0.42
2:B:389:THR:HB	2:B:843:ILE:HG13	2.01	0.42
2:B:892:VAL:HG21	2:B:897:ARG:HA	2.01	0.42
1:A:127:MET:HG3	1:A:128:PRO:CD	2.44	0.42
1:A:665:ALA:O	1:A:669:LYS:HB3	2.19	0.42
1:A:642:ILE:H	1:A:642:ILE:HG13	1.45	0.42
2:B:719:TYR:CE2	2:B:728:VAL:HA	2.54	0.42
3:C:8:ALA:HB3	3:C:41:PHE:CD1	2.54	0.42
1:A:58:PRO:HB3	1:A:119:TYR:CE1	2.55	0.42
1:A:388:ARG:HA	1:A:391:THR:HG23	2.02	0.42
1:A:607:PHE:C	1:A:609:ARG:H	2.27	0.42
2:B:876:SER:HA	2:B:1091:VAL:HG13	2.00	0.42
3:C:53:THR:O	3:C:151:ALA:HA	2.18	0.42
1:A:362:CYS:HA	1:A:365:ASN:HB2	2.02	0.42
2:B:375:ASP:O	2:B:378:LYS:HG2	2.19	0.42
2:B:446:ASP:C	2:B:448:ARG:N	2.75	0.42
1:A:131:PHE:CE2	1:A:158:LEU:HD22	2.54	0.42
1:A:638:ASP:C	1:A:640:SER:N	2.75	0.42
2:B:509:VAL:HB	2:B:636:VAL:HG22	2.01	0.42
2:B:628:SER:N	2:B:629:PRO:HD2	2.34	0.42
2:B:1084:LEU:HD23	2:B:1084:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:HG23	1:A:516:SER:HB3	2.02	0.42
3:C:38:LYS:HA	3:C:41:PHE:CD2	2.53	0.42
3:C:55:GLU:N	3:C:151:ALA:HB1	2.34	0.42
1:A:675:MET:HA	1:A:676:PRO:HD3	1.93	0.42
2:B:848:ALA:O	2:B:852:VAL:HG23	2.20	0.42
1:A:570:PHE:HD1	1:A:570:PHE:HA	1.64	0.42
3:C:151:ALA:O	3:C:152:ASN:HB2	2.19	0.42
2:B:500:PRO:HG3	3:C:18:ALA:HB3	2.02	0.41
2:B:631:GLY:HA2	2:B:685:VAL:HG22	2.02	0.41
2:B:1054:VAL:O	2:B:1056:ARG:N	2.53	0.41
1:A:73:LEU:HD12	1:A:86:ASN:ND2	2.34	0.41
1:A:185:LYS:HE2	1:A:185:LYS:HB2	1.87	0.41
1:A:508:THR:OG1	1:A:509:GLN:N	2.53	0.41
1:A:551:ILE:O	1:A:555:GLN:HG3	2.20	0.41
1:A:662:GLU:H	1:A:662:GLU:HG2	1.57	0.41
2:B:450:TRP:CE2	2:B:459:ASN:HB3	2.56	0.41
2:B:1005:LEU:O	2:B:1010:GLY:N	2.53	0.41
2:B:957:ALA:HB3	2:B:965:ILE:HB	2.03	0.41
1:A:325:LYS:H	1:A:325:LYS:HG2	1.49	0.41
2:B:348:LEU:H	2:B:348:LEU:HG	1.80	0.41
1:A:548:ARG:HG3	1:A:552:ARG:HD2	2.02	0.41
2:B:387:ARG:HD2	2:B:935:LEU:HD22	2.03	0.41
2:B:450:TRP:NE1	2:B:459:ASN:HB3	2.36	0.41
2:B:950:ASP:HA	2:B:1004:PHE:CE1	2.55	0.41
2:B:972:GLN:HB3	2:B:1071:GLU:OE1	2.21	0.41
2:B:981:ASP:HA	2:B:999:ASN:O	2.21	0.41
1:A:71:ASN:HB3	1:A:498:THR:HG21	2.03	0.41
1:A:509:GLN:O	1:A:510:ILE:C	2.64	0.41
2:B:1057:ASP:H	2:B:1060:PRO:CG	2.33	0.40
2:B:952:LEU:HD23	2:B:952:LEU:HA	1.85	0.40
1:A:689:VAL:O	1:A:693:GLN:HG3	2.20	0.40
2:B:654:GLU:OE2	2:B:696:TYR:HB2	2.20	0.40
1:A:658:ILE:HD13	1:A:688:PRO:HB2	2.02	0.40
2:B:1078:LEU:HB3	2:B:1082:GLU:HB2	2.03	0.40
1:A:17:VAL:HG23	1:A:42:PHE:HD1	1.86	0.40
2:B:437:TYR:HB2	2:B:804:GLN:NE2	2.37	0.40
2:B:700:ALA:HA	2:B:924:ILE:HG21	2.03	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	702/765 (92%)	631 (90%)	67 (10%)	4 (1%)	21	42
2	B	724/747 (97%)	658 (91%)	57 (8%)	9 (1%)	10	23
3	C	125/157 (80%)	106 (85%)	18 (14%)	1 (1%)	16	34
All	All	1551/1669 (93%)	1395 (90%)	142 (9%)	14 (1%)	14	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1056	ARG
3	C	152	ASN
2	B	961	SER
1	A	255	PRO
2	B	1055	ILE
1	A	698	SER
2	B	581	PRO
2	B	746	GLU
2	B	1060	PRO
1	A	748	SER
2	B	494	SER
2	B	565	PRO
1	A	52	PRO
2	B	1020	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	611/666 (92%)	534 (87%)	77 (13%)	4	9
2	B	648/678 (96%)	542 (84%)	106 (16%)	2	4
3	C	113/138 (82%)	103 (91%)	10 (9%)	9	21
4	D	1/1 (100%)	1 (100%)	0	100	100
All	All	1373/1483 (93%)	1180 (86%)	193 (14%)	3	6

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	17	VAL
1	A	20	SER
1	A	60	LEU
1	A	62	SER
1	A	73	LEU
1	A	76	VAL
1	A	82	LEU
1	A	129	LEU
1	A	138	CYS
1	A	154	SER
1	A	181	GLU
1	A	183	ILE
1	A	184	SER
1	A	185	LYS
1	A	236	ILE
1	A	243	LEU
1	A	247	LEU
1	A	261	LEU
1	A	263	SER
1	A	264	SER
1	A	268	LEU
1	A	270	ILE
1	A	300	MET
1	A	310	ILE
1	A	324	VAL
1	A	325	LYS
1	A	326	LYS
1	A	328	THR
1	A	332	GLU
1	A	344	VAL
1	A	352	LEU
1	A	355	THR

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Mol	Chain	Res	Type
1	A	372	VAL
1	A	376	SER
1	A	393	ASP
1	A	400	MET
1	A	427	ASN
1	A	436	ASN
1	A	438	ILE
1	A	444	CYS
1	A	454	THR
1	A	476	ARG
1	A	488	SER
1	A	498	THR
1	A	499	ILE
1	A	505	ASP
1	A	510	ILE
1	A	533	ARG
1	A	543	LEU
1	A	544	ARG
1	A	559	GLU
1	A	566	SER
1	A	570	PHE
1	A	573	THR
1	A	596	SER
1	A	612	LEU
1	A	622	ILE
1	A	623	LEU
1	A	636	LEU
1	A	642	ILE
1	A	658	ILE
1	A	662	GLU
1	A	668	ARG
1	A	669	LYS
1	A	677	GLU
1	A	680	ASN
1	A	683	HIS
1	A	695	ILE
1	A	696	LEU
1	A	709	GLU
1	A	719	LEU
1	A	722	VAL
1	A	747	VAL
1	A	748	SER

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Mol	Chain	Res	Type
1	A	753	MET
1	A	756	LEU
2	B	348	LEU
2	B	365	LEU
2	B	377	GLN
2	B	391	THR
2	B	402	LYS
2	B	410	LEU
2	B	411	LEU
2	B	414	PHE
2	B	422	VAL
2	B	424	THR
2	B	433	SER
2	B	435	ARG
2	B	443	SER
2	B	445	LEU
2	B	447	GLN
2	B	459	ASN
2	B	461	VAL
2	B	491	MET
2	B	495	GLU
2	B	512	VAL
2	B	522	LEU
2	B	523	ASN
2	B	525	VAL
2	B	529	LEU
2	B	533	LEU
2	B	554	HIS
2	B	561	SER
2	B	566	GLN
2	B	568	LEU
2	B	571	SER
2	B	573	ILE
2	B	586	VAL
2	B	588	LEU
2	B	594	LEU
2	B	602	LEU
2	B	610	LEU
2	B	612	THR
2	B	627	MET
2	B	630	THR
2	B	640	GLN

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Mol	Chain	Res	Type
2	B	644	LEU
2	B	646	VAL
2	B	659	SER
2	B	666	MET
2	B	667	THR
2	B	689	LEU
2	B	692	LEU
2	B	697	SER
2	B	707	ARG
2	B	712	SER
2	B	726	VAL
2	B	732	GLN
2	B	733	LYS
2	B	743	ILE
2	B	746	GLU
2	B	748	VAL
2	B	749	MET
2	B	751	ILE
2	B	755	LYS
2	B	771	THR
2	B	773	LEU
2	B	779	VAL
2	B	787	VAL
2	B	789	MET
2	B	794	SER
2	B	795	LEU
2	B	798	THR
2	B	807	LEU
2	B	812	SER
2	B	815	GLU
2	B	830	THR
2	B	831	LEU
2	B	854	ARG
2	B	897	ARG
2	B	909	GLN
2	B	914	THR
2	B	936	VAL
2	B	938	LEU
2	B	940	LEU
2	B	946	LEU
2	B	947	TYR
2	B	954	ASP

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Mol	Chain	Res	Type
2	B	960	ILE
2	B	967	GLN
2	B	980	ARG
2	B	994	LEU
2	B	996	VAL
2	B	999	ASN
2	B	1002	GLN
2	B	1008	VAL
2	B	1009	LEU
2	B	1011	VAL
2	B	1027	LEU
2	B	1034	ARG
2	B	1046	ARG
2	B	1048	PHE
2	B	1051	ILE
2	B	1052	LEU
2	B	1053	TYR
2	B	1054	VAL
2	B	1059	SER
2	B	1061	MET
2	B	1066	LEU
2	B	1075	GLU
2	B	1089	GLN
2	B	1093	LYS
3	C	4	LEU
3	C	23	ASP
3	C	42	ARG
3	C	44	LEU
3	C	72	LEU
3	C	111	SER
3	C	121	LYS
3	C	149	MET
3	C	150	VAL
3	C	152	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	A	354	GLN
1	A	509	GLN
1	A	549	GLN

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Mol	Chain	Res	Type
1	A	591	GLN
1	A	683	HIS
1	A	686	GLN
1	A	693	GLN
1	A	714	GLN
2	B	564	GLN
2	B	583	ASN
2	B	760	HIS
2	B	780	ASN
2	B	913	GLN
2	B	917	ASN
2	B	932	ASN
2	B	1002	GLN
2	B	1003	ASN
2	B	1064	ASN
2	B	1067	GLN
3	C	152	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	SEP	D	1	4	9,10,10	1.56	2 (22%)	12,14,14	1.65	3 (25%)

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	SEP	D	1	4	-	4/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	SEP	P-O1P	3.26	1.61	1.50
4	D	1	SEP	OXT-C	-2.17	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	SEP	P-OG-CB	-3.28	109.26	118.30
4	D	1	SEP	OG-CB-CA	2.74	110.44	108.06
4	D	1	SEP	OXT-C-O	-2.47	118.47	124.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	SEP	N-CA-CB-OG
4	D	1	SEP	CB-OG-P-O1P
4	D	1	SEP	CB-OG-P-O2P
4	D	1	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	712/765 (93%)	-0.18	4 (0%) 85 83	58, 83, 122, 224	0
2	B	732/747 (97%)	-0.22	8 (1%) 78 74	30, 79, 118, 144	0
3	C	131/157 (83%)	0.09	1 (0%) 82 80	72, 108, 151, 169	0
4	D	1/2 (50%)	0.50	0 100 100	110, 110, 110, 110	0
All	All	1576/1671 (94%)	-0.17	13 (0%) 82 80	30, 83, 127, 224	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1060	PRO	4.6
2	B	958	LEU	3.0
2	B	960	ILE	2.9
2	B	1055	ILE	2.8
1	A	667	TRP	2.8
2	B	1014	TYR	2.7
3	C	78	ALA	2.5
1	A	66	CYS	2.4
1	A	440	THR	2.2
2	B	1054	VAL	2.2
2	B	1057	ASP	2.2
1	A	700	PHE	2.1
2	B	1048	PHE	2.1

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

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(\AA^2)	Q<0.9
4	SEP	D	1	11/11	0.85	0.10	122,125,128,148	0

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(\AA^2)	Q<0.9
5	ZN	A	801	1/1	0.88	0.15	201,201,201,201	0
5	ZN	B	1101	1/1	0.99	0.03	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.