



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:12 AM UTC

PDB ID : 8SUO / pdb_00008suo
Title : BA.2/AZD1061/AZD3152 structure analysis
Authors : Oganessian, V.; van Dyk, N.; Dippel, A.; Barnes, A.; O'Connor, E.
Deposited on : 2023-05-12
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
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

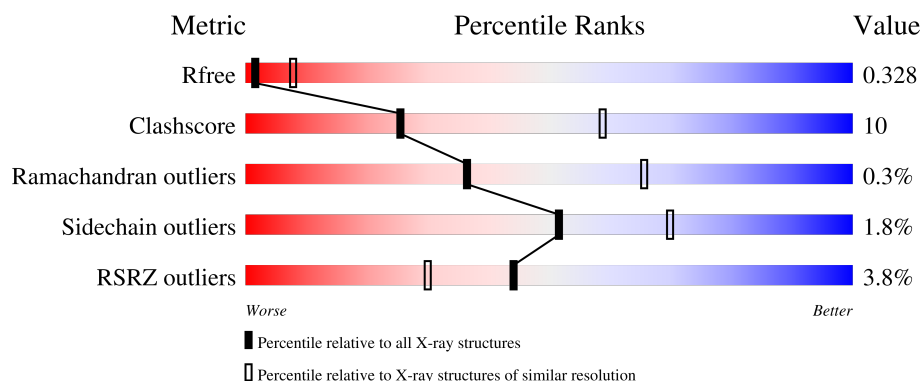
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

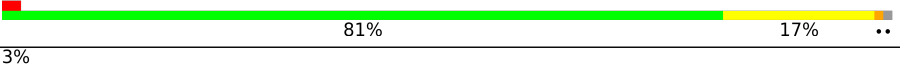
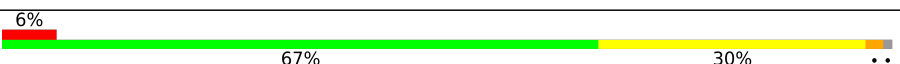
The reported resolution of this entry is 3.30 Å.

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	I	234	
2	M	219	
3	H	228	
4	L	215	
5	A	195	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8175 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 AZD1061 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	228	Total	C	N	O	S	0	0	0
			1709	1083	284	335	7			

- Molecule 2 is a protein called AZD1061 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	217	Total	C	N	O	S	0	0	0
			1676	1051	279	340	6			

- Molecule 3 is a protein called AZD3152 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	223	Total	C	N	O	S	0	0	0
			1670	1059	279	326	6			

- Molecule 4 is a protein called AZD3152 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1570	980	261	323	6			

- Molecule 5 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	194	Total	C	N	O	S	0	0	0
			1550	1002	261	279	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	PHE	SER	conflict	UNP P0DTC2

Continued on next page...

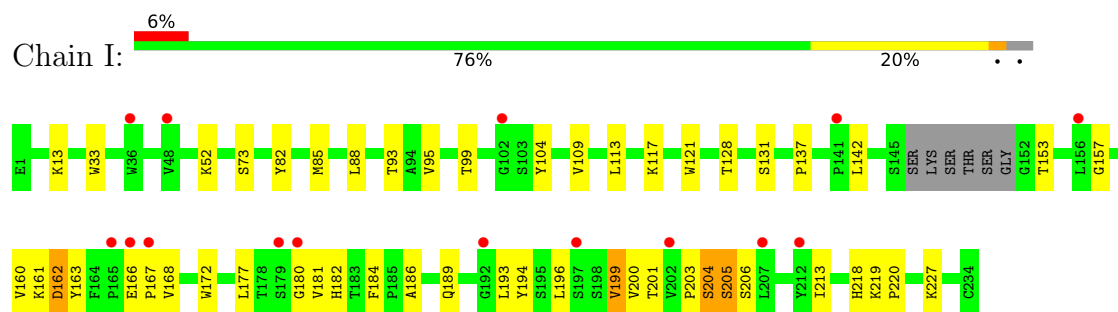
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	376	ALA	THR	conflict	UNP P0DTC2
A	405	ASN	ASP	conflict	UNP P0DTC2
A	408	SER	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2
A	493	ARG	GLN	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2

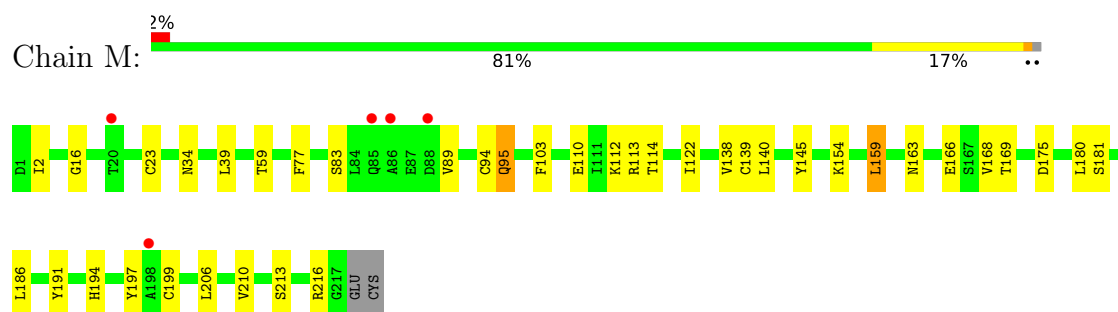
3 Residue-property plots [i](#)

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.

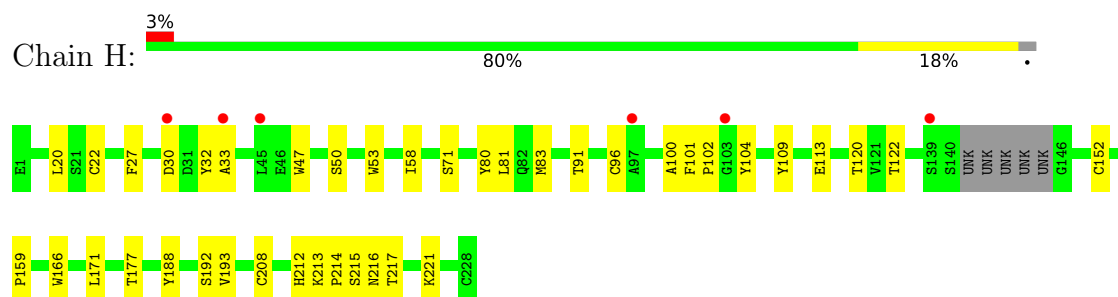
- Molecule 1: AZD1061 heavy chain



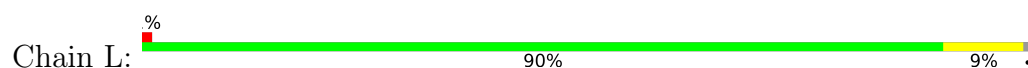
- Molecule 2: AZD1061 light chain

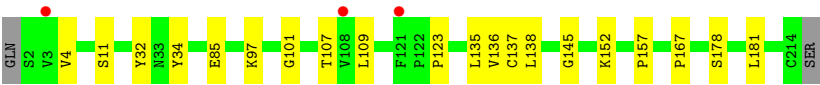


- Molecule 3: AZD3152 heavy chain

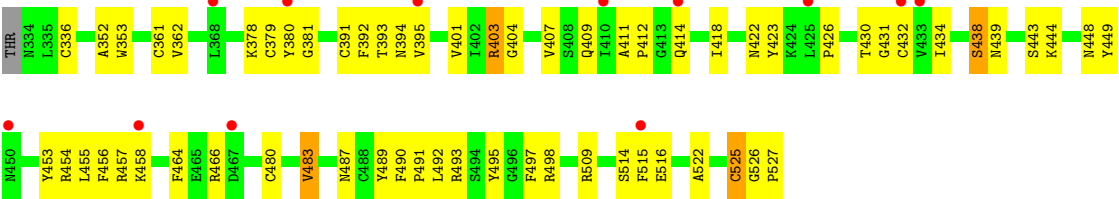


- Molecule 4: AZD3152 light chain





● Molecule 5: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.69Å 138.00Å 188.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.5 (30.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.279 , 0.332 0.279 , 0.328	Depositor DCC
R_{free} test set	1866 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8175	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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](#)

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	I	0.46	0/1751	0.75	0/2383
2	M	0.46	0/1712	0.72	0/2324
3	H	0.48	0/1714	0.75	0/2335
4	L	0.50	0/1608	0.78	0/2192
5	A	0.45	0/1598	0.74	0/2175
All	All	0.47	0/8383	0.75	0/11409

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	I	1709	0	1681	39	0
2	M	1676	0	1631	28	0
3	H	1670	0	1624	31	0
4	L	1570	0	1519	14	0
5	A	1550	0	1481	44	0
All	All	8175	0	7936	144	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 10.

All (144) 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:I:153:THR:HA	1:I:203:PRO:HA	1.47	0.96
3:H:22:CYS:HG	3:H:96:CYS:HG	1.20	0.89
4:L:152:LYS:HA	4:L:157:PRO:HA	1.54	0.87
2:M:23:CYS:HG	2:M:94:CYS:HG	1.01	0.83
5:A:336:CYS:HG	5:A:361:CYS:HG	0.82	0.80
2:M:139:CYS:HG	2:M:199:CYS:HG	1.03	0.80
5:A:391:CYS:HG	5:A:525:CYS:HG	1.20	0.79
5:A:379:CYS:HA	5:A:432:CYS:HA	1.70	0.73
4:L:137:CYS:O	4:L:138:LEU:HD23	1.88	0.72
3:H:20:LEU:HD11	3:H:83:MET:HE2	1.71	0.72
5:A:401:VAL:HG22	5:A:509:ARG:HG2	1.75	0.67
1:I:160:VAL:HG11	1:I:168:VAL:HG21	1.79	0.65
1:I:13:LYS:HD3	1:I:131:SER:HA	1.79	0.65
3:H:213:LYS:N	3:H:214:PRO:HD2	2.13	0.64
1:I:168:VAL:HG12	1:I:218:HIS:HB2	1.81	0.63
2:M:16:GLY:HA2	2:M:83:SER:HB2	1.82	0.61
5:A:455:LEU:HD23	5:A:456:PHE:HD2	1.66	0.60
1:I:163:TYR:HE1	1:I:166:GLU:HA	1.67	0.60
5:A:379:CYS:HG	5:A:432:CYS:HG	1.46	0.59
2:M:206:LEU:HD13	2:M:210:VAL:HG12	1.84	0.59
3:H:22:CYS:HG	3:H:96:CYS:CB	2.16	0.58
1:I:184:PHE:CE1	2:M:169:THR:HG23	2.38	0.58
1:I:99:THR:HG1	1:I:121:TRP:CD1	2.21	0.58
2:M:139:CYS:CB	2:M:199:CYS:HG	2.18	0.57
1:I:189:GLN:HE21	1:I:193:LEU:HB2	1.69	0.57
1:I:204:SER:O	1:I:205:SER:C	2.48	0.57
1:I:153:THR:CA	1:I:203:PRO:HA	2.31	0.56
3:H:166:TRP:HB3	3:H:171:LEU:HD23	1.87	0.56
3:H:50:SER:O	3:H:58:ILE:HA	2.06	0.56
5:A:391:CYS:CB	5:A:525:CYS:HG	2.18	0.55
5:A:418:ILE:HA	5:A:422:ASN:HB2	1.86	0.55
2:M:191:TYR:HA	2:M:197:TYR:OH	2.06	0.55
5:A:454:ARG:HA	5:A:492:LEU:HD23	1.88	0.55
1:I:157:GLY:HA3	1:I:199:VAL:HA	1.88	0.55
2:M:168:VAL:HG22	2:M:180:LEU:HD13	1.88	0.55
5:A:380:TYR:O	5:A:431:GLY:N	2.40	0.55
5:A:422:ASN:O	5:A:423:TYR:HB3	2.06	0.54
3:H:159:PRO:HD2	3:H:214:PRO:HB3	1.89	0.54
4:L:4:VAL:HB	4:L:101:GLY:HA2	1.89	0.53
5:A:403:ARG:HG2	5:A:495:TYR:HE2	1.72	0.53
3:H:212:HIS:CE1	3:H:214:PRO:HB2	2.43	0.53
4:L:137:CYS:C	4:L:138:LEU:HD23	2.32	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:TYR:O	5:A:444:LYS:HD3	2.09	0.52
5:A:453:TYR:HB3	5:A:495:TYR:CE1	2.44	0.52
4:L:135:LEU:HD12	4:L:181:LEU:HD23	1.91	0.51
2:M:113:ARG:NH1	2:M:114:THR:O	2.43	0.51
3:H:101:PHE:CE2	5:A:455:LEU:HD21	2.45	0.51
5:A:392:PHE:CD2	5:A:515:PHE:HB3	2.46	0.51
2:M:166:GLU:HB3	2:M:180:LEU:HD11	1.93	0.51
3:H:152:CYS:SG	3:H:208:CYS:CB	2.98	0.51
1:I:219:LYS:N	1:I:220:PRO:CD	2.74	0.51
3:H:100:ALA:HB2	3:H:113:GLU:HB2	1.92	0.51
3:H:213:LYS:N	3:H:214:PRO:CD	2.75	0.50
2:M:154:LYS:HG2	2:M:159:LEU:HA	1.94	0.50
3:H:177:THR:HG22	3:H:192:SER:OG	2.12	0.50
1:I:162:ASP:HA	1:I:193:LEU:HB3	1.94	0.50
1:I:199:VAL:HG21	2:M:140:LEU:HD13	1.94	0.49
3:H:20:LEU:HD12	3:H:81:LEU:O	2.11	0.49
2:M:194:HIS:O	2:M:216:ARG:NH2	2.44	0.49
3:H:215:SER:O	3:H:216:ASN:HB2	2.12	0.49
3:H:177:THR:HA	3:H:192:SER:HA	1.94	0.49
5:A:439:ASN:O	5:A:443:SER:HB2	2.11	0.49
1:I:104:TYR:HE1	1:I:109:VAL:HG23	1.78	0.49
1:I:93:THR:HG23	1:I:128:THR:HA	1.96	0.48
2:M:166:GLU:HA	2:M:181:SER:O	2.14	0.48
3:H:193:VAL:HG21	4:L:138:LEU:HD12	1.95	0.48
3:H:20:LEU:HD11	3:H:83:MET:CE	2.43	0.48
3:H:109:TYR:HA	4:L:34:TYR:HB3	1.94	0.48
2:M:89:VAL:HG12	2:M:110:GLU:HA	1.96	0.48
5:A:362:VAL:HB	5:A:526:GLY:HA2	1.96	0.48
3:H:102:PRO:O	5:A:457:ARG:O	2.32	0.47
1:I:180:GLY:HA3	1:I:201:THR:HG22	1.96	0.47
5:A:426:PRO:HD3	5:A:464:PHE:CE2	2.49	0.47
3:H:159:PRO:HA	3:H:188:TYR:HE2	1.77	0.47
1:I:162:ASP:OD1	1:I:189:GLN:NE2	2.48	0.47
5:A:412:PRO:HB3	5:A:426:PRO:O	2.14	0.47
5:A:448:ASN:HB3	5:A:497:PHE:HB2	1.97	0.47
2:M:95:GLN:HB2	2:M:103:PHE:CD2	2.50	0.46
3:H:215:SER:OG	3:H:217:THR:HB	2.16	0.46
5:A:381:GLY:HA3	5:A:430:THR:HA	1.95	0.46
1:I:186:ALA:HB2	1:I:196:LEU:HD23	1.98	0.46
2:M:112:LYS:HA	2:M:145:TYR:OH	2.15	0.46
4:L:123:PRO:HD3	4:L:135:LEU:CD2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:393:THR:HA	5:A:522:ALA:HA	1.98	0.46
5:A:455:LEU:HD23	5:A:456:PHE:CD2	2.46	0.46
5:A:490:PHE:CG	5:A:491:PRO:HD2	2.50	0.46
4:L:145:GLY:O	4:L:167:PRO:HG2	2.16	0.46
1:I:166:GLU:HG2	1:I:167:PRO:HA	1.99	0.45
4:L:85:GLU:HG3	4:L:107:THR:HA	1.99	0.45
1:I:157:GLY:CA	1:I:199:VAL:HA	2.46	0.45
1:I:204:SER:O	1:I:206:SER:N	2.49	0.45
1:I:142:LEU:HD21	2:M:138:VAL:HG21	1.99	0.45
3:H:22:CYS:SG	3:H:96:CYS:CB	3.05	0.45
4:L:138:LEU:HD22	4:L:178:SER:HB3	1.98	0.45
1:I:186:ALA:HA	1:I:196:LEU:HB3	1.99	0.45
2:M:122:ILE:HD12	2:M:213:SER:HA	1.98	0.45
5:A:353:TRP:CD1	5:A:423:TYR:HB2	2.52	0.44
5:A:394:ASN:HB2	5:A:516:GLU:OE1	2.17	0.44
5:A:404:GLY:HA2	5:A:407:VAL:HG23	2.00	0.44
2:M:34:ASN:HD22	5:A:449:TYR:CB	2.31	0.44
1:I:142:LEU:CD2	2:M:138:VAL:HG21	2.48	0.44
1:I:85:MET:HB3	1:I:88:LEU:HD21	1.98	0.43
3:H:91:THR:HG23	3:H:122:THR:HA	1.99	0.43
5:A:526:GLY:N	5:A:527:PRO:HD3	2.32	0.43
2:M:39:LEU:HD13	2:M:77:PHE:CG	2.54	0.43
1:I:113:LEU:HD13	1:I:117:LYS:C	2.43	0.43
4:L:11:SER:HB2	4:L:109:LEU:HD11	2.00	0.43
5:A:409:GLN:HA	5:A:414:GLN:OE1	2.19	0.43
3:H:33:ALA:CB	3:H:104:TYR:HA	2.48	0.43
4:L:136:VAL:HG12	4:L:136:VAL:O	2.18	0.43
5:A:401:VAL:CG2	5:A:509:ARG:HG2	2.46	0.43
2:M:39:LEU:HD13	2:M:77:PHE:CD1	2.54	0.43
3:H:213:LYS:O	3:H:214:PRO:C	2.62	0.43
1:I:181:VAL:O	1:I:182:HIS:HD2	2.02	0.42
1:I:180:GLY:H	1:I:200:VAL:HG23	1.84	0.42
5:A:480:CYS:O	5:A:483:VAL:HG22	2.18	0.42
3:H:47:TRP:CZ3	4:L:97:LYS:HB2	2.54	0.42
5:A:438:SER:OG	5:A:509:ARG:HG3	2.20	0.42
1:I:213:ILE:HA	1:I:227:LYS:O	2.20	0.42
2:M:139:CYS:HG	2:M:199:CYS:CB	2.31	0.42
5:A:395:VAL:HA	5:A:514:SER:O	2.19	0.42
1:I:137:PRO:HA	1:I:162:ASP:O	2.19	0.41
5:A:449:TYR:OH	5:A:498:ARG:NH2	2.53	0.41
2:M:34:ASN:HD22	5:A:449:TYR:HB3	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:27:PHE:HD2	3:H:32:TYR:CD2	2.38	0.41
3:H:212:HIS:HD1	3:H:215:SER:CB	2.32	0.41
1:I:172:TRP:HB3	1:I:177:LEU:HD23	2.02	0.41
2:M:163:ASN:OD1	2:M:163:ASN:N	2.54	0.41
1:I:163:TYR:H	1:I:194:TYR:H	1.68	0.41
2:M:186:LEU:HD23	2:M:186:LEU:HA	1.95	0.41
3:H:30:ASP:O	3:H:53:TRP:HB2	2.21	0.41
1:I:162:ASP:HB3	1:I:193:LEU:HD13	2.03	0.41
5:A:487:ASN:HA	5:A:489:TYR:CZ	2.56	0.41
1:I:161:LYS:HG2	1:I:162:ASP:OD1	2.21	0.41
5:A:411:ALA:HB3	5:A:414:GLN:HB2	2.03	0.40
1:I:33:TRP:CH2	1:I:52:LYS:HD2	2.57	0.40
1:I:73:SER:HB2	1:I:82:TYR:HB2	2.03	0.40
3:H:71:SER:OG	3:H:80:TYR:HB2	2.22	0.40
5:A:378:LYS:HD2	5:A:380:TYR:CZ	2.56	0.40
5:A:453:TYR:CZ	5:A:493:ARG:HB3	2.56	0.40
1:I:137:PRO:HA	1:I:163:TYR:HB3	2.04	0.40
2:M:122:ILE:HD11	2:M:199:CYS:CB	2.52	0.40
5:A:352:ALA:HA	5:A:466:ARG:HD3	2.03	0.40
5:A:379:CYS:CB	5:A:432:CYS:HG	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	224/234 (96%)	204 (91%)	17 (8%)	3 (1%)	9	35
2	M	215/219 (98%)	199 (93%)	16 (7%)	0	100	100
3	H	219/228 (96%)	202 (92%)	17 (8%)	0	100	100
4	L	211/215 (98%)	197 (93%)	14 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	192/195 (98%)	170 (88%)	22 (12%)	0	100	100
All	All	1061/1091 (97%)	972 (92%)	86 (8%)	3 (0%)	36	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	205	SER
1	I	204	SER
1	I	162	ASP

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	I	190/195 (97%)	188 (99%)	2 (1%)	65	76
2	M	190/192 (99%)	185 (97%)	5 (3%)	40	64
3	H	184/184 (100%)	182 (99%)	2 (1%)	65	76
4	L	177/179 (99%)	176 (99%)	1 (1%)	78	81
5	A	166/167 (99%)	160 (96%)	6 (4%)	31	58
All	All	907/917 (99%)	891 (98%)	16 (2%)	51	70

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	95	VAL
1	I	199	VAL
2	M	2	ILE
2	M	59	THR
2	M	95	GLN
2	M	159	LEU
2	M	175	ASP
3	H	120	THR
3	H	221	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	32	TYR
5	A	403	ARG
5	A	434	ILE
5	A	438	SER
5	A	458	LYS
5	A	483	VAL
5	A	525	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	182	HIS
1	I	189	GLN
1	I	210	GLN
2	M	34	ASN
2	M	48	GLN
2	M	85	GLN
4	L	33	ASN
4	L	41	HIS
4	L	197	GLN
5	A	405	ASN
5	A	487	ASN
5	A	505	HIS

5.3.3 RNA [i](#)

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](#)

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](#)

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	I	228/234 (97%)	0.46	15 (6%) 24 16	78, 122, 154, 174	0
2	M	217/219 (99%)	0.23	5 (2%) 61 42	74, 126, 149, 184	0
3	H	223/228 (97%)	0.32	6 (2%) 56 37	37, 110, 142, 166	0
4	L	213/215 (99%)	0.16	3 (1%) 73 55	30, 104, 134, 210	0
5	A	194/195 (99%)	0.48	12 (6%) 26 18	105, 152, 230, 272	0
All	All	1075/1091 (98%)	0.33	41 (3%) 44 30	30, 121, 190, 272	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	86	ALA	6.7
1	I	167	PRO	4.4
5	A	410	ILE	4.2
5	A	414	GLN	4.0
3	H	33	ALA	4.0
5	A	450	ASN	3.9
1	I	166	GLU	3.5
1	I	197	SER	3.2
3	H	30	ASP	3.1
1	I	102	GLY	3.1
3	H	103	GLY	2.9
1	I	202	VAL	2.9
5	A	368	LEU	2.8
3	H	45	LEU	2.8
5	A	395	VAL	2.7
5	A	432	CYS	2.7
5	A	425	LEU	2.6
3	H	97	ALA	2.6
1	I	212	TYR	2.5
2	M	88	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	180	GLY	2.4
1	I	192	GLY	2.4
5	A	380	TYR	2.3
1	I	36	TRP	2.3
1	I	156	LEU	2.3
3	H	139	SER	2.2
5	A	467	ASP	2.2
2	M	20	THR	2.2
5	A	458	LYS	2.2
1	I	179	SER	2.1
1	I	48	VAL	2.1
1	I	165	PRO	2.1
2	M	85	GLN	2.1
1	I	141	PRO	2.1
4	L	108	VAL	2.1
2	M	198	ALA	2.1
4	L	121	PHE	2.1
1	I	207	LEU	2.0
5	A	515	PHE	2.0
5	A	433	VAL	2.0
4	L	3	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.