



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:05 PM UTC

PDB ID : 8FSL / pdb_00008fsl
Title : Human Mesothelin bound to a neutralizing VH domain antibody
Authors : Calero, G.
Deposited on : 2023-01-10
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

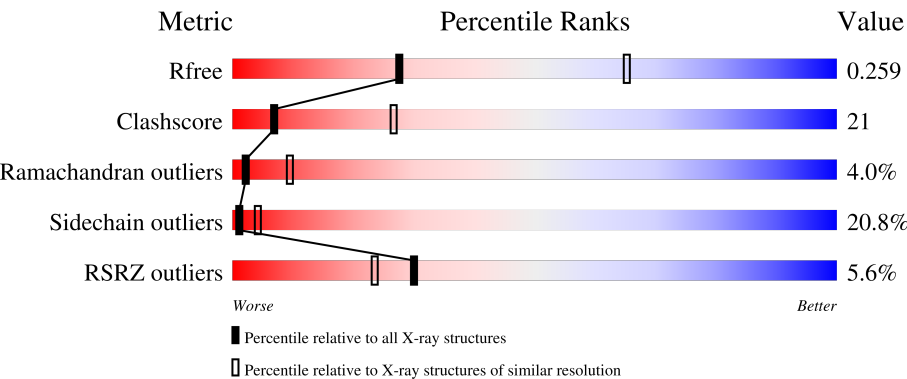
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	116	3% 57% 37% • •
1	B	116	22% 38% 46% 11% 5%
1	C	116	3% 40% 46% 14% •
1	D	116	11% 35% 36% 11% • 16%
2	E	285	% 62% 29% 8% •

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Mol	Chain	Length	Quality of chain
2	F	285	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', followed by a green segment labeled '50%', a yellow segment labeled '35%', and a small orange segment at the end labeled '12%'. A small grey dot is visible at the far right end of the bar.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7817 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 VH domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	Se	0	0	0
			882	553	155	170	2	2			
1	C	115	Total	C	N	O	S	Se	0	0	0
			880	551	153	172	2	2			
1	D	98	Total	C	N	O	S	Se	0	0	0
			763	480	134	145	2	2			
1	B	110	Total	C	N	O	S	Se	0	0	0
			853	535	151	163	2	2			

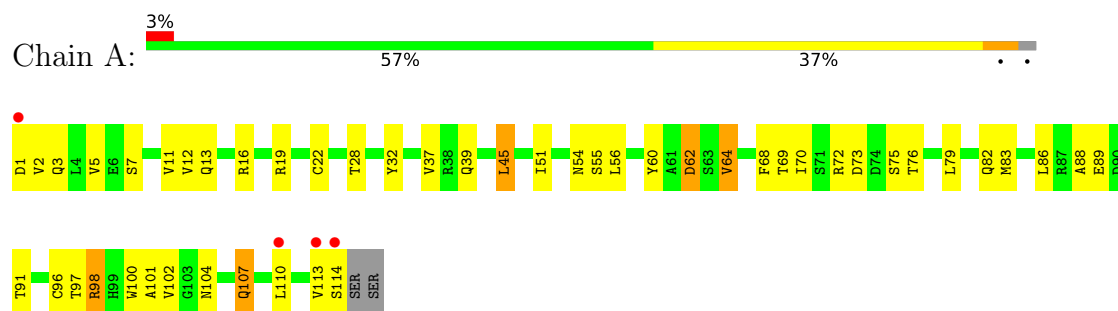
- Molecule 2 is a protein called Mesothelin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	285	Total	C	N	O	S	0	0	0
			2240	1429	376	426	9			
2	F	278	Total	C	N	O	S	0	0	0
			2199	1405	368	417	9			

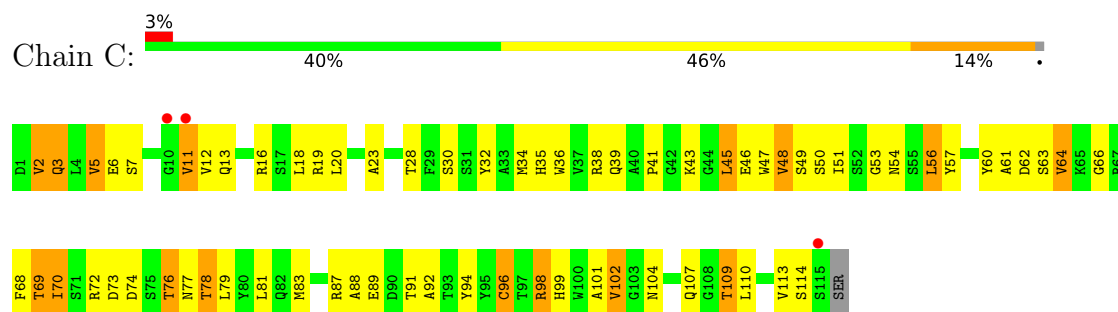
3 Residue-property plots [i](#)

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.

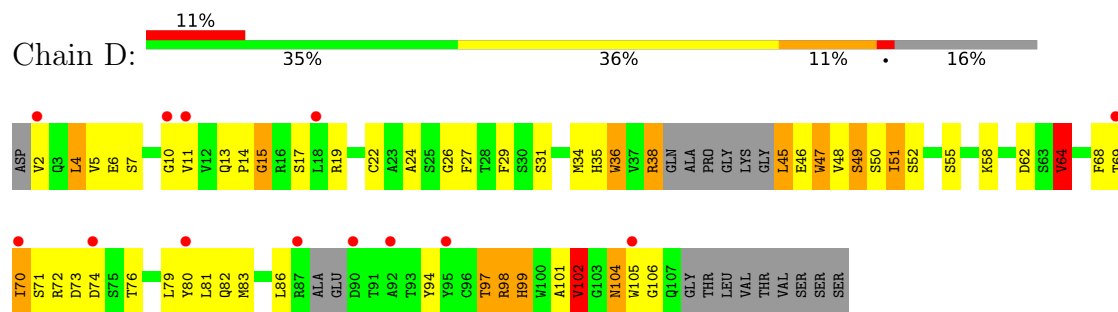
• Molecule 1: VH domain



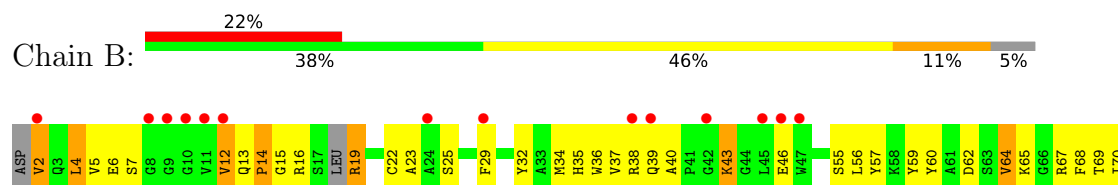
• Molecule 1: VH domain

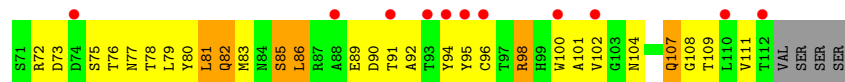


• Molecule 1: VH domain

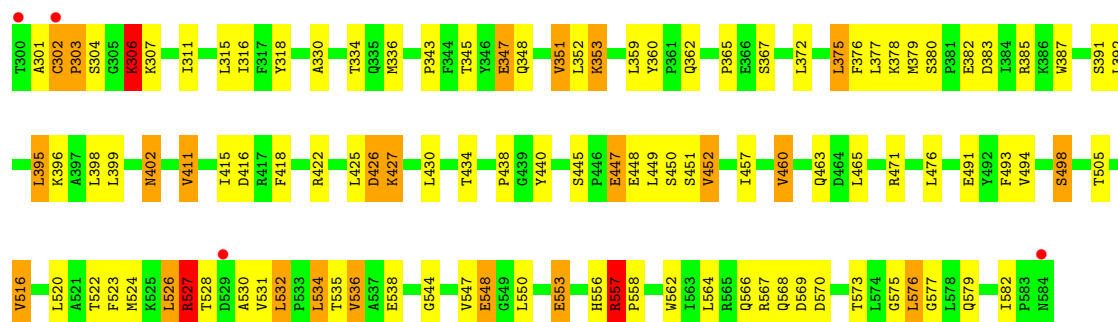


• Molecule 1: VH domain

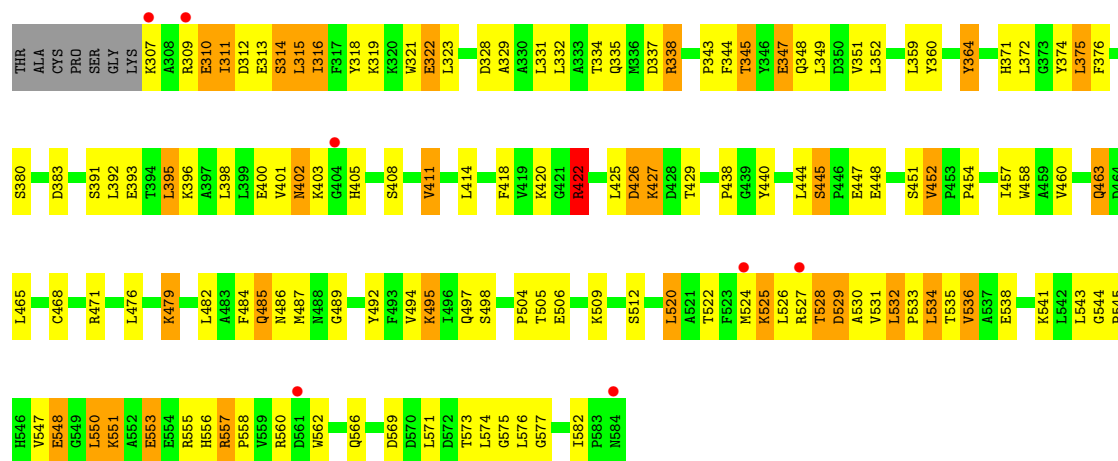




● Molecule 2: Mesothelin



● Molecule 2: Mesothelin



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.12Å 114.12Å 340.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.90 39.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.90-2.90) 99.9 (39.90-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158_4158, PHENIX 1.19.2-4158_4158	Depositor
R, R_{free}	0.238 , 0.254 0.242 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å ²)	101.4	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7817	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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	A	0.61	0/901	0.85	0/1220
1	B	0.43	0/871	0.73	0/1177
1	C	0.46	0/899	0.77	0/1218
1	D	0.37	0/779	0.62	0/1051
2	E	0.52	0/2288	0.81	2/3109 (0.1%)
2	F	0.44	0/2246	0.73	3/3051 (0.1%)
All	All	0.48	0/7984	0.76	5/10826 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	556	HIS	N-CA-C	8.38	121.92	110.35
2	F	422	ARG	N-CA-C	-8.16	104.47	114.75
2	E	556	HIS	N-CA-C	7.39	120.55	110.35
2	F	582	ILE	N-CA-C	-6.54	103.01	108.63
2	E	557	ARG	N-CA-C	5.30	121.51	109.81

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	882	0	843	26	0
1	B	853	0	810	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	880	0	830	46	0
1	D	763	0	701	46	0
2	E	2240	0	2224	73	0
2	F	2199	0	2192	100	0
All	All	7817	0	7600	326	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 21.

All (326) 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:C:64:VAL:HB	1:C:68:PHE:HD2	1.21	1.05
2:F:309:ARG:CB	2:F:331:LEU:HD22	1.89	1.01
2:F:309:ARG:HB3	2:F:331:LEU:HD22	1.01	1.00
1:C:64:VAL:HB	1:C:68:PHE:CD2	1.96	1.00
2:F:557:ARG:CB	2:F:558:PRO:CD	2.41	0.99
2:E:557:ARG:CB	2:E:558:PRO:HD3	1.97	0.94
2:E:557:ARG:CB	2:E:558:PRO:CD	2.45	0.94
2:E:523:PHE:HA	2:E:526:LEU:HD22	1.51	0.93
2:F:309:ARG:HB3	2:F:331:LEU:CD2	1.96	0.91
2:F:557:ARG:CB	2:F:558:PRO:HD3	1.98	0.90
2:E:379:MET:HE2	2:E:387:TRP:HZ2	1.39	0.88
2:F:548:GLU:HA	2:F:576:LEU:HD21	1.60	0.81
2:E:465:LEU:HD12	2:E:498:SER:HB2	1.64	0.78
1:C:2:VAL:HG13	1:C:3:GLN:H	1.48	0.78
1:D:38:ARG:HE	1:D:94:TYR:HE1	1.28	0.78
2:F:531:VAL:HA	2:F:534:LEU:HD22	1.68	0.76
1:A:88:ALA:O	1:A:91:THR:HG22	1.85	0.75
2:E:535:THR:HG23	2:E:538:GLU:H	1.53	0.74
1:D:73:ASP:HB3	1:D:76:THR:HG22	1.70	0.74
1:B:12:VAL:HG22	1:B:16:ARG:HH21	1.53	0.73
2:E:302:CYS:H	2:E:303:PRO:HD3	1.54	0.73
1:D:13:GLN:O	1:D:15:GLY:N	2.22	0.72
2:F:345:THR:HG22	2:F:348:GLN:H	1.54	0.71
1:B:83:MSE:HE2	1:B:86:LEU:HD12	1.72	0.71
2:E:379:MET:HE2	2:E:387:TRP:CZ2	2.25	0.70
2:F:309:ARG:HD3	2:F:328:ASP:HB3	1.73	0.70
2:F:535:THR:HG23	2:F:538:GLU:H	1.55	0.69
1:C:20:LEU:HD11	1:C:94:TYR:HD2	1.56	0.69
2:F:574:LEU:HB3	2:F:576:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:MET:HE3	2:E:383:ASP:HB3	1.75	0.69
1:B:68:PHE:HE2	1:B:83:MSE:HE3	1.56	0.69
1:B:83:MSE:SE	1:B:94:TYR:HE2	2.26	0.69
1:D:101:ALA:HB1	1:D:104:ASN:HB2	1.75	0.68
1:B:29:PHE:CE2	1:B:72:ARG:HG3	2.29	0.68
2:F:312:ASP:OD1	2:F:314:SER:HB3	1.93	0.67
2:E:536:VAL:HG21	2:E:570:ASP:HB3	1.77	0.67
1:D:49:SER:OG	1:D:70:ILE:HG12	1.95	0.66
1:D:71:SER:HB2	1:D:80:TYR:HB2	1.76	0.66
2:E:330:ALA:HA	2:E:359:LEU:HD11	1.77	0.66
1:C:38:ARG:HG3	1:C:94:TYR:HE1	1.61	0.66
1:D:97:THR:OG1	1:D:98:ARG:N	2.27	0.66
1:B:40:ALA:HB1	1:B:43:LYS:HD3	1.78	0.65
2:F:426:ASP:OD1	2:F:427:LYS:N	2.29	0.65
2:F:562:TRP:O	2:F:566:GLN:HG2	1.96	0.65
1:B:29:PHE:HE2	1:B:72:ARG:CG	2.10	0.65
2:F:392:LEU:HG	2:F:422:ARG:HH12	1.62	0.64
1:C:6:GLU:OE2	1:C:96:CYS:N	2.25	0.64
1:D:51:ILE:HD12	1:D:55:SER:HA	1.78	0.64
1:B:64:VAL:HG13	1:B:68:PHE:CD1	2.33	0.64
2:F:457:ILE:O	2:F:460:VAL:HG12	1.99	0.63
2:F:524:MET:CE	2:F:557:ARG:CB	2.76	0.63
1:D:6:GLU:OE1	1:B:108:GLY:N	2.31	0.63
1:B:68:PHE:CE2	1:B:83:MSE:HE3	2.32	0.63
2:F:524:MET:SD	2:F:553:GLU:HG2	2.39	0.62
2:F:398:LEU:O	2:F:401:VAL:HG12	1.99	0.62
2:E:527:ARG:HB2	2:E:530:ALA:HB3	1.82	0.62
2:F:311:ILE:HA	2:F:315:LEU:HD23	1.81	0.61
1:C:32:TYR:OH	2:E:378:LYS:NZ	2.33	0.61
1:D:99:HIS:CD2	1:D:101:ALA:H	2.18	0.61
1:D:34:MSE:HB3	1:D:79:LEU:HD11	1.81	0.61
2:F:307:LYS:HA	2:F:318:TYR:OH	2.00	0.61
1:B:55:SER:OG	1:B:72:ARG:HD2	2.01	0.60
1:B:34:MSE:HB3	1:B:79:LEU:HD22	1.84	0.60
1:A:13:GLN:HB2	1:A:16:ARG:HD3	1.83	0.60
1:A:32:TYR:O	1:A:72:ARG:NH2	2.35	0.59
2:F:309:ARG:HD3	2:F:328:ASP:CB	2.32	0.59
2:F:529:ASP:OD1	2:F:529:ASP:N	2.31	0.59
2:E:302:CYS:H	2:E:303:PRO:CD	2.15	0.59
2:E:505:THR:OG1	2:E:530:ALA:O	2.20	0.59
1:B:76:THR:O	1:B:78:THR:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:VAL:HG22	1:B:68:PHE:CE1	2.37	0.58
1:C:68:PHE:HE1	1:C:83:MSE:SE	2.36	0.58
1:D:104:ASN:ND2	1:B:98:ARG:HD3	2.19	0.58
1:D:104:ASN:HD21	1:B:98:ARG:HD3	1.69	0.58
2:E:567:ARG:HH21	2:E:569:ASP:HB2	1.69	0.57
1:D:98:ARG:NH1	1:B:104:ASN:OD1	2.33	0.57
2:F:487:MET:HE3	2:F:492:TYR:HA	1.86	0.57
1:B:85:SER:O	1:B:85:SER:OG	2.16	0.57
1:A:113:VAL:HG11	1:C:88:ALA:HA	1.85	0.57
2:F:524:MET:HE3	2:F:557:ARG:CB	2.34	0.57
2:F:319:LYS:HB2	2:F:322:GLU:HG3	1.86	0.57
2:E:402:ASN:OD1	2:E:402:ASN:N	2.36	0.56
2:F:536:VAL:HG13	2:F:562:TRP:HH2	1.70	0.56
2:F:524:MET:HE1	2:F:557:ARG:CB	2.34	0.56
2:F:359:LEU:HD23	2:F:360:TYR:CE2	2.41	0.56
1:B:29:PHE:CE2	1:B:72:ARG:CG	2.87	0.56
1:B:70:ILE:HD11	1:B:79:LEU:HD11	1.88	0.56
1:C:45:LEU:HD12	1:C:45:LEU:H	1.69	0.56
1:D:4:LEU:HD12	1:D:24:ALA:HB2	1.86	0.56
2:F:376:PHE:CD2	2:F:398:LEU:HD22	2.40	0.56
2:F:497:GLN:HE21	2:F:522:THR:HG21	1.71	0.56
1:D:35:HIS:CD2	1:D:102:VAL:HG21	2.41	0.56
2:E:524:MET:SD	2:E:553:GLU:HG2	2.46	0.55
1:B:68:PHE:CD2	1:B:83:MSE:HG2	2.41	0.55
2:F:319:LYS:HB2	2:F:322:GLU:CG	2.35	0.55
1:B:89:GLU:CD	1:B:89:GLU:H	2.13	0.55
2:F:551:LYS:HG3	2:F:576:LEU:O	2.06	0.55
1:C:61:ALA:O	1:C:64:VAL:HG22	2.06	0.55
2:E:360:TYR:CD1	2:E:365:PRO:HD3	2.42	0.55
1:D:98:ARG:NH2	2:F:347:GLU:OE2	2.39	0.55
1:B:40:ALA:CB	1:B:43:LYS:HD3	2.36	0.55
1:D:45:LEU:HD13	1:D:46:GLU:N	2.22	0.55
1:A:51:ILE:HD11	1:A:55:SER:HA	1.89	0.55
1:A:102:VAL:HG23	2:E:343:PRO:O	2.06	0.54
1:C:51:ILE:HB	1:C:70:ILE:HD12	1.89	0.54
1:C:76:THR:O	1:C:78:THR:N	2.40	0.54
2:F:402:ASN:OD1	2:F:402:ASN:N	2.41	0.54
1:B:107:GLN:H	1:B:107:GLN:CD	2.15	0.54
1:C:73:ASP:OD2	1:C:76:THR:HG23	2.08	0.54
2:E:524:MET:CE	2:E:553:GLU:HG2	2.38	0.54
1:D:36:TRP:CH2	1:D:79:LEU:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ASP:OD1	1:B:76:THR:N	2.29	0.53
2:E:345:THR:HG23	2:E:348:GLN:H	1.73	0.53
1:B:4:LEU:N	1:B:4:LEU:HD23	2.23	0.53
1:C:83:MSE:SE	1:C:94:TYR:HE2	2.40	0.53
2:F:535:THR:HG22	2:F:538:GLU:CD	2.33	0.53
2:F:438:PRO:C	2:F:440:TYR:H	2.16	0.53
2:F:484:PHE:CE1	2:F:495:LYS:HG2	2.43	0.53
1:C:39:GLN:NE2	1:C:43:LYS:O	2.41	0.53
2:E:380:SER:O	2:E:383:ASP:HB2	2.09	0.52
2:F:426:ASP:O	2:F:427:LYS:HB2	2.10	0.52
1:D:48:VAL:HG12	1:D:49:SER:HB3	1.91	0.52
2:F:307:LYS:CB	2:F:318:TYR:OH	2.58	0.52
1:B:22:CYS:O	1:B:78:THR:HA	2.10	0.52
1:B:29:PHE:CZ	1:B:72:ARG:HG3	2.45	0.51
2:E:426:ASP:OD1	2:E:427:LYS:N	2.42	0.51
1:B:107:GLN:HG2	1:B:108:GLY:H	1.75	0.51
1:A:64:VAL:HG13	1:A:68:PHE:HB2	1.93	0.51
2:E:527:ARG:HB3	2:E:530:ALA:H	1.75	0.51
1:B:2:VAL:N	1:B:25:SER:O	2.44	0.51
1:B:39:GLN:O	1:B:92:ALA:HB1	2.09	0.51
2:E:445:SER:O	2:E:447:GLU:N	2.44	0.51
2:F:452:VAL:O	2:F:479:LYS:HE3	2.11	0.51
1:A:19:ARG:HE	1:A:82:GLN:HG2	1.76	0.51
1:D:98:ARG:O	1:D:98:ARG:HG2	2.11	0.51
2:F:463:GLN:H	2:F:463:GLN:CD	2.18	0.51
2:F:575:GLY:O	2:F:577:GLY:N	2.39	0.51
2:E:575:GLY:O	2:E:577:GLY:N	2.39	0.51
2:F:418:PHE:HE1	2:F:422:ARG:HH11	1.59	0.50
2:E:430:LEU:O	2:E:434:THR:HG23	2.12	0.50
1:B:37:VAL:HG13	1:B:46:GLU:O	2.10	0.50
1:A:54:ASN:OD1	1:A:56:LEU:HB2	2.12	0.50
2:F:349:LEU:HD23	2:F:352:LEU:HD12	1.94	0.50
2:E:568:GLN:O	2:E:568:GLN:NE2	2.33	0.50
1:C:98:ARG:HH22	2:E:347:GLU:CD	2.20	0.50
2:F:426:ASP:OD2	2:F:429:THR:OG1	2.27	0.50
2:F:520:LEU:O	2:F:524:MET:HG2	2.11	0.50
1:B:5:VAL:O	1:B:22:CYS:HA	2.11	0.50
1:B:83:MSE:HE1	1:B:94:TYR:OH	2.11	0.50
1:D:64:VAL:HG22	1:D:68:PHE:CE2	2.47	0.50
1:D:83:MSE:HE2	1:D:86:LEU:HD21	1.94	0.49
1:A:101:ALA:HB3	1:A:104:ASN:HD21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ARG:CG	1:C:94:TYR:HE1	2.26	0.49
2:E:471:ARG:HG2	2:E:471:ARG:HH11	1.77	0.49
1:D:99:HIS:CD2	1:D:101:ALA:HB3	2.48	0.49
1:C:68:PHE:CE1	1:C:83:MSE:SE	3.16	0.49
2:E:535:THR:HG22	2:E:538:GLU:CD	2.37	0.49
1:C:88:ALA:O	1:C:91:THR:HG22	2.13	0.49
1:D:22:CYS:HB3	1:D:79:LEU:HB2	1.94	0.49
1:D:101:ALA:HB1	1:D:104:ASN:CB	2.41	0.49
1:C:38:ARG:NE	1:C:46:GLU:OE2	2.33	0.48
2:E:535:THR:HG23	2:E:538:GLU:N	2.27	0.48
2:F:505:THR:OG1	2:F:530:ALA:O	2.26	0.48
2:E:348:GLN:O	2:E:352:LEU:HD13	2.12	0.48
2:E:562:TRP:O	2:E:566:GLN:HG2	2.13	0.48
1:C:34:MSE:HB3	1:C:79:LEU:HD22	1.96	0.48
2:E:445:SER:O	2:E:448:GLU:N	2.46	0.48
2:E:330:ALA:HA	2:E:359:LEU:CD1	2.43	0.47
2:E:523:PHE:O	2:E:526:LEU:HB2	2.13	0.47
2:F:426:ASP:CG	2:F:429:THR:H	2.22	0.47
1:B:36:TRP:NE1	1:B:81:LEU:HB2	2.28	0.47
1:B:60:TYR:CZ	1:B:70:ILE:HG22	2.49	0.47
2:E:527:ARG:HA	2:E:527:ARG:HD3	1.65	0.47
2:E:532:LEU:HD13	2:E:532:LEU:HA	1.70	0.47
2:F:312:ASP:HA	1:B:59:TYR:HE2	1.80	0.47
2:F:458:TRP:CZ3	2:F:495:LYS:HE3	2.49	0.47
1:B:19:ARG:HB3	1:B:82:GLN:OE1	2.15	0.47
1:C:38:ARG:HB3	1:C:46:GLU:HG3	1.96	0.47
2:E:457:ILE:O	2:E:460:VAL:HG13	2.15	0.47
1:B:60:TYR:OH	1:B:70:ILE:HG22	2.15	0.47
2:E:306:LYS:HG2	2:E:307:LYS:O	2.15	0.47
2:F:445:SER:O	2:F:447:GLU:N	2.47	0.47
2:F:311:ILE:O	2:F:311:ILE:HG22	2.15	0.46
2:E:348:GLN:O	2:E:351:VAL:HG13	2.15	0.46
1:B:36:TRP:CD1	1:B:81:LEU:HB2	2.50	0.46
2:E:544:GLY:O	2:E:547:VAL:HG23	2.15	0.46
1:D:34:MSE:SE	1:D:98:ARG:HB2	2.65	0.46
2:E:382:GLU:HG3	2:E:385:ARG:HH22	1.81	0.46
2:F:485:GLN:H	2:F:485:GLN:HG3	1.49	0.46
2:F:532:LEU:HD13	2:F:532:LEU:HA	1.71	0.46
2:F:313:GLU:HB3	1:B:59:TYR:HD2	1.81	0.46
2:E:359:LEU:HD22	2:E:360:TYR:CE2	2.51	0.46
2:E:476:LEU:HD23	2:E:476:LEU:HA	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:372:LEU:HD22	2:E:375:LEU:HB3	1.98	0.46
2:E:547:VAL:HG12	2:E:576:LEU:HD21	1.98	0.46
2:F:343:PRO:O	1:B:102:VAL:HG23	2.15	0.46
1:D:17:SER:HB2	1:D:83:MSE:O	2.16	0.46
2:F:403:LYS:O	2:F:405:HIS:ND1	2.45	0.46
1:A:39:GLN:HB2	1:A:45:LEU:CD1	2.46	0.45
1:C:5:VAL:HG13	1:C:23:ALA:HB3	1.98	0.45
1:C:36:TRP:NE1	1:C:81:LEU:HB2	2.31	0.45
2:F:550:LEU:HD12	2:F:550:LEU:HA	1.83	0.45
1:C:38:ARG:HG3	1:C:94:TYR:CE1	2.47	0.45
1:C:99:HIS:NE2	1:C:101:ALA:HB3	2.32	0.45
2:E:376:PHE:CD2	2:E:398:LEU:HD22	2.52	0.45
2:E:524:MET:CE	2:E:557:ARG:CB	2.94	0.45
1:B:83:MSE:HE2	1:B:86:LEU:CD1	2.43	0.45
1:C:60:TYR:CE2	1:C:69:THR:HA	2.51	0.45
1:D:83:MSE:HE1	1:D:94:TYR:HE2	1.82	0.45
1:B:22:CYS:N	1:B:79:LEU:O	2.49	0.45
1:B:29:PHE:HE2	1:B:72:ARG:HG2	1.81	0.45
1:D:69:THR:HB	1:D:82:GLN:HB2	1.98	0.45
2:E:395:LEU:HD22	2:E:399:LEU:HG	1.98	0.45
1:C:13:GLN:HB2	1:C:16:ARG:HG3	1.98	0.45
2:F:395:LEU:HG	2:F:418:PHE:CD2	2.52	0.45
2:F:364:TYR:N	2:F:364:TYR:CD1	2.85	0.45
2:F:484:PHE:CZ	2:F:495:LYS:HG2	2.52	0.45
1:A:68:PHE:CE2	1:A:83:MSE:HG2	2.53	0.45
2:F:310:GLU:OE1	2:F:310:GLU:HA	2.17	0.45
1:D:58:LYS:HB3	1:D:70:ILE:CD1	2.47	0.44
1:D:99:HIS:HD2	1:D:102:VAL:H	1.63	0.44
2:F:307:LYS:CA	2:F:318:TYR:OH	2.65	0.44
2:F:374:TYR:HE1	1:B:32:TYR:HE1	1.64	0.44
2:F:465:LEU:O	2:F:468:CYS:HB2	2.18	0.44
1:B:6:GLU:HG2	1:B:95:TYR:HA	1.99	0.44
2:F:372:LEU:O	2:F:375:LEU:HB2	2.18	0.44
1:C:64:VAL:HB	1:C:68:PHE:CE2	2.47	0.44
2:E:491:GLU:O	2:E:494:VAL:HG12	2.18	0.44
2:F:522:THR:HA	2:F:525:LYS:HE2	1.99	0.44
1:B:70:ILE:HG13	1:B:80:TYR:O	2.17	0.44
1:C:89:GLU:H	1:C:89:GLU:CD	2.24	0.44
1:D:83:MSE:HE1	1:D:94:TYR:CE2	2.52	0.44
1:A:73:ASP:OD1	1:A:76:THR:N	2.46	0.44
2:F:557:ARG:CB	2:F:558:PRO:HD2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TRP:O	1:C:48:VAL:HG13	2.18	0.44
2:E:396:LYS:HB2	2:E:396:LYS:HE3	1.71	0.44
2:F:484:PHE:HB3	2:F:487:MET:HE2	1.99	0.44
2:F:332:LEU:HD22	2:F:352:LEU:HD22	2.00	0.43
2:F:505:THR:HG21	2:F:533:PRO:HG2	1.99	0.43
1:D:35:HIS:NE2	1:D:102:VAL:HG21	2.33	0.43
2:F:566:GLN:HB2	2:F:571:LEU:HD21	2.00	0.43
2:E:531:VAL:HA	2:E:534:LEU:HD22	1.99	0.43
2:F:329:ALA:HB3	2:F:359:LEU:HD13	2.00	0.43
2:F:504:PRO:HB2	2:F:506:GLU:OE1	2.18	0.43
2:E:449:LEU:O	2:E:452:VAL:HG13	2.18	0.43
2:F:316:ILE:HG22	2:F:344:PHE:HA	2.01	0.43
2:F:338:ARG:NH1	1:B:57:TYR:OH	2.52	0.43
2:F:380:SER:O	2:F:383:ASP:HB2	2.19	0.43
1:D:68:PHE:CZ	1:D:83:MSE:HE3	2.54	0.43
1:A:2:VAL:O	1:A:2:VAL:HG13	2.18	0.43
2:F:425:LEU:HD23	2:F:425:LEU:HA	1.77	0.43
1:A:13:GLN:HB2	1:A:16:ARG:CD	2.49	0.42
1:D:105:TRP:HA	1:B:4:LEU:HD11	2.01	0.42
2:E:353:LYS:HD2	2:E:353:LYS:C	2.44	0.42
2:E:418:PHE:CE1	2:E:422:ARG:HD2	2.54	0.42
1:C:35:HIS:ND1	1:C:50:SER:OG	2.37	0.42
1:D:105:TRP:CA	1:B:4:LEU:HD21	2.49	0.42
1:A:7:SER:HA	1:C:109:THR:HG21	2.02	0.42
2:E:426:ASP:O	2:E:427:LYS:HB2	2.20	0.42
2:F:316:ILE:H	2:F:316:ILE:HG12	1.64	0.42
2:E:345:THR:HG22	2:E:348:GLN:CG	2.50	0.42
2:E:524:MET:HE3	2:E:524:MET:HB3	1.81	0.42
2:F:338:ARG:NH1	1:B:57:TYR:CZ	2.87	0.42
1:A:62:ASP:C	1:A:64:VAL:H	2.27	0.42
2:E:382:GLU:HG3	2:E:385:ARG:NH2	2.35	0.42
2:E:425:LEU:O	2:E:427:LYS:N	2.52	0.42
2:E:493:PHE:CD1	2:E:516:VAL:HG21	2.55	0.42
2:F:543:LEU:HD23	2:F:543:LEU:HA	1.83	0.42
2:F:322:GLU:H	2:F:322:GLU:HG2	1.60	0.42
2:F:374:TYR:CE1	1:B:32:TYR:HE1	2.37	0.42
1:B:4:LEU:HD23	1:B:4:LEU:H	1.83	0.42
1:D:36:TRP:CZ3	1:D:81:LEU:HB2	2.55	0.42
1:D:35:HIS:CD2	1:D:50:SER:OG	2.72	0.42
1:D:47:TRP:HZ3	1:D:50:SER:HG	1.68	0.42
1:D:52:SER:O	1:D:72:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASN:OD1	1:C:56:LEU:HB2	2.20	0.42
1:D:2:VAL:N	1:D:26:GLY:HA3	2.35	0.42
2:E:336:MET:HE1	2:E:375:LEU:HD12	2.02	0.42
2:E:411:VAL:O	2:E:415:ILE:HG13	2.20	0.42
2:E:535:THR:O	2:E:538:GLU:N	2.53	0.42
2:F:348:GLN:O	2:F:351:VAL:HG12	2.20	0.42
1:B:13:GLN:HA	1:B:14:PRO:HD3	1.93	0.42
1:A:88:ALA:HA	1:C:113:VAL:HB	2.02	0.41
1:C:53:GLY:HA2	1:C:72:ARG:NH2	2.34	0.41
2:F:311:ILE:HA	2:F:315:LEU:CD2	2.46	0.41
1:A:113:VAL:H	1:C:91:THR:HB	1.86	0.41
1:C:70:ILE:HG23	1:C:81:LEU:CD1	2.50	0.41
1:D:29:PHE:C	1:D:31:SER:H	2.27	0.41
1:A:5:VAL:O	1:A:22:CYS:HA	2.20	0.41
1:C:62:ASP:C	1:C:64:VAL:H	2.27	0.41
2:F:311:ILE:HB	2:F:335:GLN:OE1	2.20	0.41
2:F:318:TYR:HB2	2:F:323:LEU:HD13	2.01	0.41
2:E:306:LYS:HE2	2:E:318:TYR:CZ	2.54	0.41
2:E:392:LEU:HD23	2:E:392:LEU:HA	1.85	0.41
2:E:524:MET:HE3	2:E:557:ARG:CB	2.50	0.41
2:E:548:GLU:H	2:E:548:GLU:HG3	1.50	0.41
2:F:512:SER:O	2:F:541:LYS:HG2	2.21	0.41
2:F:528:THR:C	2:F:530:ALA:N	2.78	0.41
2:F:345:THR:HG23	2:F:347:GLU:HG2	2.03	0.41
1:D:106:GLY:N	1:B:6:GLU:OE2	2.37	0.41
2:F:337:ASP:HA	2:F:371:HIS:HB3	2.02	0.41
1:B:4:LEU:HA	1:B:23:ALA:O	2.20	0.41
1:A:60:TYR:OH	1:A:70:ILE:HG22	2.20	0.41
1:A:98:ARG:H	1:A:98:ARG:HG2	1.66	0.41
1:C:20:LEU:CD1	1:C:94:TYR:HD2	2.28	0.41
2:F:411:VAL:HA	2:F:414:LEU:HB3	2.03	0.41
2:F:476:LEU:HD23	2:F:476:LEU:HA	1.83	0.41
2:E:304:SER:HB3	2:E:307:LYS:H	1.86	0.41
2:E:438:PRO:C	2:E:440:TYR:H	2.28	0.41
2:F:544:GLY:O	2:F:547:VAL:HG23	2.20	0.41
1:C:2:VAL:HG13	1:C:3:GLN:N	2.26	0.40
1:B:101:ALA:HB3	1:B:104:ASN:HD21	1.86	0.40
1:A:97:THR:OG1	1:A:98:ARG:N	2.53	0.40
1:C:56:LEU:HB3	1:C:57:TYR:CD1	2.56	0.40
1:C:83:MSE:SE	1:C:94:TYR:CE2	3.24	0.40
1:A:89:GLU:H	1:A:89:GLU:CD	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLN:CD	1:A:107:GLN:H	2.30	0.40
1:D:72:ARG:HD3	1:D:74:ASP:OD1	2.21	0.40
2:F:438:PRO:C	2:F:440:TYR:N	2.80	0.40
2:F:505:THR:OG1	2:F:530:ALA:HA	2.22	0.40
1:A:68:PHE:CD2	1:A:83:MSE:HG2	2.56	0.40
1:C:41:PRO:HD3	1:C:92:ALA:HA	2.02	0.40
1:C:66:GLY:HA3	2:F:545:PRO:HB3	2.03	0.40
1:D:73:ASP:CB	1:D:76:THR:HG22	2.48	0.40
2:F:445:SER:O	2:F:448:GLU:N	2.55	0.40
2:F:454:PRO:HG3	2:F:482:LEU:HD23	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	112/116 (97%)	104 (93%)	7 (6%)	1 (1%)	14	41
1	B	106/116 (91%)	89 (84%)	11 (10%)	6 (6%)	1	4
1	C	113/116 (97%)	95 (84%)	10 (9%)	8 (7%)	1	2
1	D	92/116 (79%)	73 (79%)	12 (13%)	7 (8%)	1	2
2	E	283/285 (99%)	249 (88%)	24 (8%)	10 (4%)	3	12
2	F	276/285 (97%)	242 (88%)	27 (10%)	7 (2%)	4	17
All	All	982/1034 (95%)	852 (87%)	91 (9%)	39 (4%)	2	9

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	VAL
1	C	77	ASN

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Mol	Chain	Res	Type
1	C	102	VAL
1	C	114	SER
1	D	7	SER
1	D	99	HIS
2	E	302	CYS
2	E	303	PRO
2	E	426	ASP
2	E	527	ARG
2	E	528	THR
2	E	557	ARG
2	F	426	ASP
2	F	427	LYS
2	F	527	ARG
2	F	557	ARG
1	B	77	ASN
1	B	91	THR
1	D	14	PRO
1	D	64	VAL
2	E	301	ALA
2	E	306	LYS
2	E	427	LYS
1	B	90	ASP
1	C	3	GLN
1	D	15	GLY
1	C	11	VAL
1	C	28	THR
1	D	10	GLY
2	F	528	THR
1	B	7	SER
1	A	28	THR
2	E	311	ILE
2	F	444	LEU
1	B	15	GLY
1	D	102	VAL
1	C	12	VAL
1	B	14	PRO
2	F	489	GLY

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	94/94 (100%)	76 (81%)	18 (19%)	1	5
1	B	90/94 (96%)	66 (73%)	24 (27%)	0	1
1	C	93/94 (99%)	67 (72%)	26 (28%)	0	1
1	D	79/94 (84%)	61 (77%)	18 (23%)	1	3
2	E	244/250 (98%)	205 (84%)	39 (16%)	2	8
2	F	241/250 (96%)	191 (79%)	50 (21%)	1	4
All	All	841/876 (96%)	666 (79%)	175 (21%)	1	4

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	3	GLN
1	A	11	VAL
1	A	12	VAL
1	A	37	VAL
1	A	45	LEU
1	A	62	ASP
1	A	64	VAL
1	A	69	THR
1	A	75	SER
1	A	79	LEU
1	A	86	LEU
1	A	96	CYS
1	A	98	ARG
1	A	100	TRP
1	A	107	GLN
1	A	110	LEU
1	A	114	SER
1	C	5	VAL
1	C	7	SER
1	C	11	VAL
1	C	18	LEU
1	C	19	ARG
1	C	30	SER
1	C	45	LEU
1	C	47	TRP

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Mol	Chain	Res	Type
1	C	48	VAL
1	C	49	SER
1	C	56	LEU
1	C	63	SER
1	C	64	VAL
1	C	69	THR
1	C	70	ILE
1	C	74	ASP
1	C	76	THR
1	C	78	THR
1	C	87	ARG
1	C	96	CYS
1	C	98	ARG
1	C	102	VAL
1	C	104	ASN
1	C	107	GLN
1	C	109	THR
1	C	110	LEU
1	D	4	LEU
1	D	5	VAL
1	D	11	VAL
1	D	19	ARG
1	D	27	PHE
1	D	36	TRP
1	D	38	ARG
1	D	45	LEU
1	D	47	TRP
1	D	49	SER
1	D	51	ILE
1	D	62	ASP
1	D	64	VAL
1	D	70	ILE
1	D	97	THR
1	D	98	ARG
1	D	102	VAL
1	D	104	ASN
2	E	306	LYS
2	E	315	LEU
2	E	316	ILE
2	E	334	THR
2	E	347	GLU
2	E	351	VAL

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Mol	Chain	Res	Type
2	E	353	LYS
2	E	362	GLN
2	E	367	SER
2	E	375	LEU
2	E	377	LEU
2	E	391	SER
2	E	395	LEU
2	E	402	ASN
2	E	411	VAL
2	E	416	ASP
2	E	447	GLU
2	E	450	SER
2	E	451	SER
2	E	452	VAL
2	E	460	VAL
2	E	463	GLN
2	E	498	SER
2	E	516	VAL
2	E	520	LEU
2	E	522	THR
2	E	526	LEU
2	E	527	ARG
2	E	532	LEU
2	E	534	LEU
2	E	536	VAL
2	E	548	GLU
2	E	550	LEU
2	E	553	GLU
2	E	564	LEU
2	E	573	THR
2	E	576	LEU
2	E	579	GLN
2	E	582	ILE
2	F	310	GLU
2	F	311	ILE
2	F	314	SER
2	F	315	LEU
2	F	316	ILE
2	F	321	TRP
2	F	322	GLU
2	F	334	THR
2	F	338	ARG

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Mol	Chain	Res	Type
2	F	345	THR
2	F	347	GLU
2	F	364	TYR
2	F	375	LEU
2	F	391	SER
2	F	393	GLU
2	F	395	LEU
2	F	396	LYS
2	F	400	GLU
2	F	402	ASN
2	F	408	SER
2	F	411	VAL
2	F	420	LYS
2	F	422	ARG
2	F	445	SER
2	F	451	SER
2	F	452	VAL
2	F	463	GLN
2	F	471	ARG
2	F	479	LYS
2	F	485	GLN
2	F	486	ASN
2	F	494	VAL
2	F	495	LYS
2	F	498	SER
2	F	509	LYS
2	F	520	LEU
2	F	525	LYS
2	F	526	LEU
2	F	529	ASP
2	F	532	LEU
2	F	534	LEU
2	F	536	VAL
2	F	548	GLU
2	F	550	LEU
2	F	551	LYS
2	F	553	GLU
2	F	555	ARG
2	F	560	ARG
2	F	569	ASP
2	F	573	THR
1	B	2	VAL

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Mol	Chain	Res	Type
1	B	4	LEU
1	B	12	VAL
1	B	19	ARG
1	B	35	HIS
1	B	38	ARG
1	B	43	LYS
1	B	56	LEU
1	B	62	ASP
1	B	64	VAL
1	B	65	LYS
1	B	67	ARG
1	B	69	THR
1	B	75	SER
1	B	81	LEU
1	B	82	GLN
1	B	85	SER
1	B	86	LEU
1	B	96	CYS
1	B	98	ARG
1	B	100	TRP
1	B	107	GLN
1	B	109	THR
1	B	111	VAL

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	82	GLN
1	A	104	ASN
1	D	35	HIS
2	E	486	ASN
2	E	556	HIS
2	F	486	ASN
2	F	497	GLN
2	F	556	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	112/116 (96%)	0.05	4 (3%)	46 38	64, 76, 130, 189	0
1	B	108/116 (93%)	1.15	25 (23%)	2 2	113, 166, 215, 229	0
1	C	113/116 (97%)	0.25	3 (2%)	56 47	72, 113, 156, 168	0
1	D	96/116 (82%)	0.81	13 (13%)	7 5	100, 142, 179, 201	0
2	E	285/285 (100%)	0.01	4 (1%)	73 65	69, 95, 133, 185	0
2	F	278/285 (97%)	0.18	7 (2%)	58 48	88, 109, 146, 174	0
All	All	992/1034 (95%)	0.29	56 (5%)	30 23	64, 107, 175, 229	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	VAL	5.4
1	D	2	VAL	5.3
1	A	114	SER	4.3
2	F	404	GLY	4.3
2	F	584	ASN	4.1
1	B	29	PHE	3.9
1	B	74	ASP	3.6
2	E	302	CYS	3.5
1	D	105	TRP	3.5
1	D	69	THR	3.5
1	D	18	LEU	3.4
2	F	561	ASP	3.2
1	C	11	VAL	3.2
1	C	115	SER	3.1
1	B	45	LEU	3.0
1	B	110	LEU	3.0
1	B	94	TYR	3.0
1	B	102	VAL	3.0
1	B	47	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	93	THR	2.9
1	B	112	THR	2.9
1	B	91	THR	2.9
1	B	38	ARG	2.8
1	D	87	ARG	2.8
1	D	90	ASP	2.8
1	B	88	ALA	2.8
1	A	110	LEU	2.8
2	E	584	ASN	2.7
1	D	92	ALA	2.6
1	D	10	GLY	2.6
1	B	39	GLN	2.6
1	D	11	VAL	2.6
1	D	80	TYR	2.5
2	E	300	THR	2.5
1	C	10	GLY	2.4
1	B	8	GLY	2.4
1	B	9	GLY	2.4
1	B	12	VAL	2.4
1	B	10	GLY	2.3
2	F	307	LYS	2.3
2	F	527	ARG	2.3
1	B	95	TYR	2.3
1	B	24	ALA	2.2
2	F	309	ARG	2.2
1	B	100	TRP	2.2
1	A	113	VAL	2.2
1	B	42	GLY	2.2
1	B	11	VAL	2.2
1	A	1	ASP	2.1
2	F	524	MET	2.1
1	B	96	CYS	2.1
2	E	529	ASP	2.1
1	D	95	TYR	2.0
1	D	70	ILE	2.0
1	D	74	ASP	2.0
1	B	46	GLU	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.