



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:08 AM EDT

PDB ID : 4XXD / pdb_00004xxd
Title : Crystal Structure of mid-region amyloid beta capture by solanezumab
Authors : Hermans, S.J.; Crespi, G.A.N.; Parker, M.W.; Miles, L.A.
Deposited on : 2015-01-30
Resolution : 2.41 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:

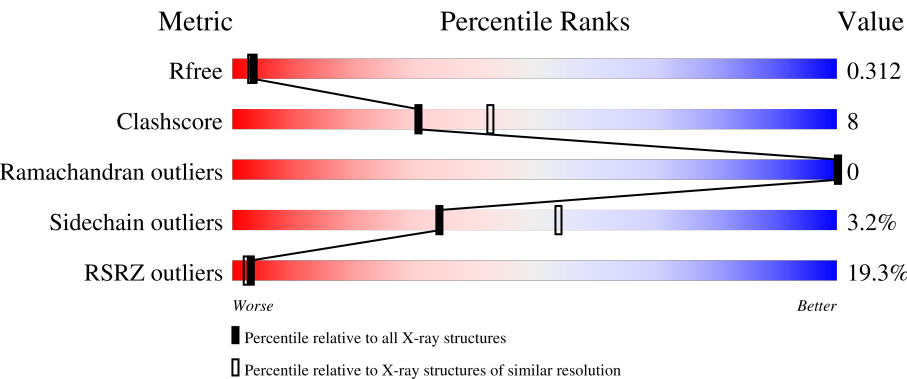
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	219	10% 84% 15% .
1	D	219	38% 69% 26% ..
2	B	223	9% 84% 9% 8%
2	E	223	17% 73% 15% 8% .
3	C	17	24% 53% 12% 35%

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Mol	Chain	Length	Quality of chain
3	F	17	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6854 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 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1686	1060	286	335	5			
1	D	217	Total	C	N	O	S	0	0	0
			1677	1055	285	332	5			

- Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	0	0
			1525	961	256	302	6			
2	E	206	Total	C	N	O	S	0	0	0
			1528	964	257	301	6			

- Molecule 3 is a protein called Amyloid-beta fragment.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			85	57	12	16			
3	F	9	Total	C	N	O	0	0	0
			75	52	10	13			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	66	Total	O	0	0
			66	66		
4	C	3	Total	O	0	0
			3	3		
4	D	56	Total	O	0	0
			56	56		

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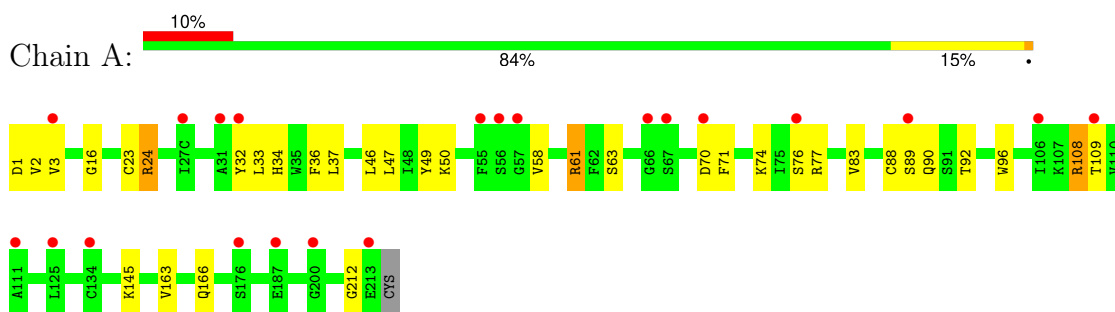
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	75	Total 75	O 75	0	0
4	F	2	Total 2	O 2	0	0

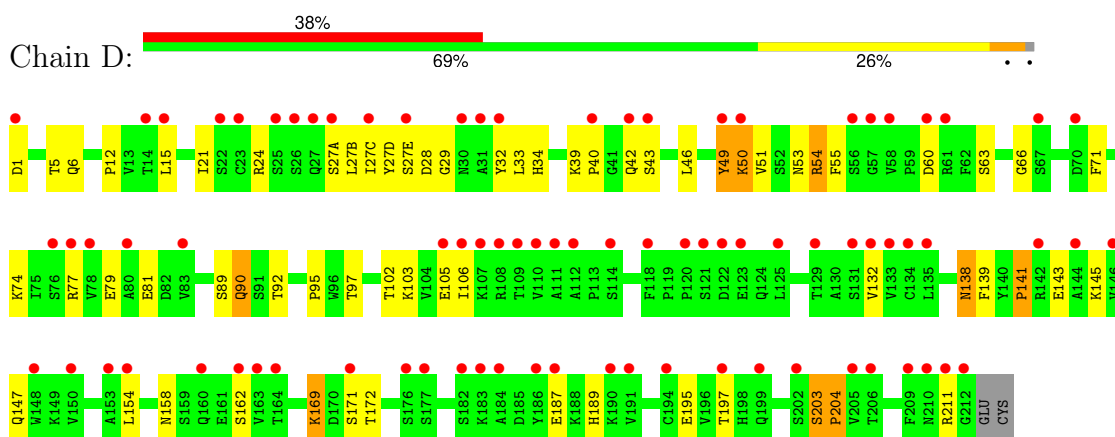
3 Residue-property plots [i](#)

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.

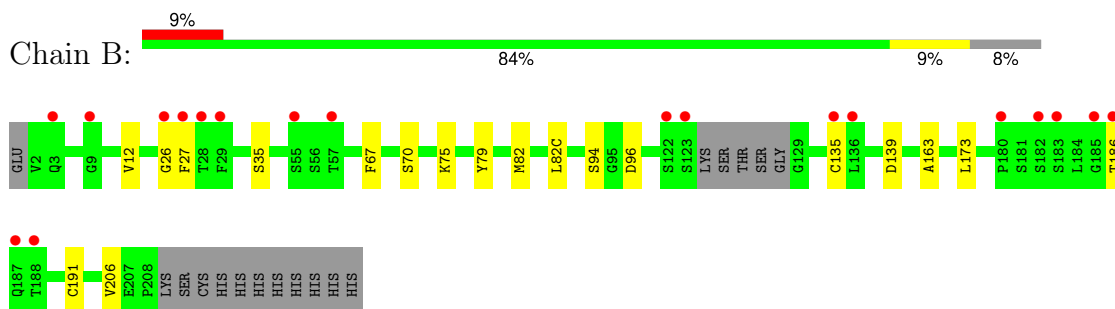
- Molecule 1: Fab Light Chain



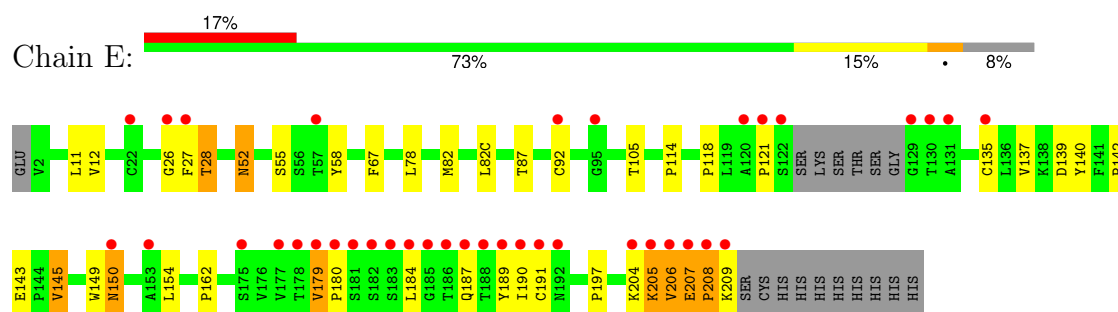
- Molecule 1: Fab Light Chain



- Molecule 2: Fab Heavy Chain



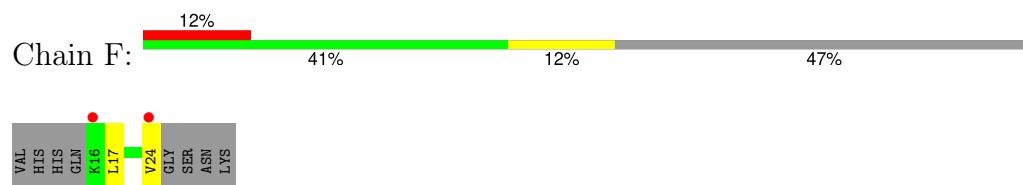
- Molecule 2: Fab Heavy Chain



- Molecule 3: Amyloid-beta fragment



- Molecule 3: Amyloid-beta fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.80Å 73.56Å 92.12Å 109.91° 93.64° 93.31°	Depositor
Resolution (Å)	46.56 – 2.41 46.56 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.56-2.41) 97.8 (46.56-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.249 , 0.290 0.266 , 0.312	Depositor DCC
R_{free} test set	1796 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.4	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	0.88	EDS
Total number of atoms	6854	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8675e-03.*

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	0.85	1/1725 (0.1%)	1.17	1/2343 (0.0%)
1	D	1.02	6/1716 (0.3%)	1.37	21/2331 (0.9%)
2	B	0.75	0/1559	1.20	9/2125 (0.4%)
2	E	0.78	1/1562 (0.1%)	1.29	14/2128 (0.7%)
3	C	0.73	0/86	1.27	0/114
3	F	0.73	0/76	1.23	0/101
All	All	0.86	8/6724 (0.1%)	1.26	45/9142 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	40	PRO	N-CD	10.01	1.61	1.47
1	A	212	GLY	C-O	-5.76	1.18	1.24
2	E	208	PRO	N-CD	5.59	1.55	1.47
1	D	203	SER	C-N	5.59	1.40	1.33
1	D	53	ASN	C-O	-5.58	1.17	1.24
1	D	50	LYS	N-CA	-5.28	1.39	1.46
1	D	6	GLN	C-O	-5.23	1.17	1.23
1	D	89	SER	C-O	-5.04	1.17	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	ASN	N-CA-C	14.09	130.28	112.24
2	B	27	PHE	N-CA-C	13.52	129.83	111.71
2	E	184	LEU	CB-CA-C	10.89	129.19	110.68
2	B	27	PHE	N-CA-CB	-9.99	96.07	111.66
1	D	50	LYS	CB-CA-C	-9.10	98.38	111.76
1	D	50	LYS	N-CA-C	8.95	124.72	107.71
2	E	179	VAL	CB-CA-C	-8.78	101.22	110.53
2	E	26	GLY	N-CA-C	8.51	127.30	114.61
1	D	139	PHE	N-CA-C	7.99	122.80	110.42
1	D	51	VAL	N-CA-CB	7.69	123.92	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	LYS	CB-CA-C	7.53	125.82	110.31
2	E	27	PHE	N-CA-C	7.51	122.51	112.30
1	D	49	TYR	N-CA-C	7.26	120.61	111.24
1	D	40	PRO	CA-N-CD	-7.18	101.94	112.00
2	B	26	GLY	N-CA-C	6.61	124.12	115.40
1	D	139	PHE	N-CA-CB	-6.48	100.45	110.56
2	E	179	VAL	N-CA-C	6.46	115.67	108.05
2	E	67	PHE	CA-CB-CG	6.26	120.06	113.80
1	D	42	GLN	N-CA-C	6.11	119.95	108.65
2	E	27	PHE	N-CA-CB	-5.93	101.64	111.49
2	E	139	ASP	N-CA-C	5.87	118.35	111.02
1	D	60	ASP	CA-C-N	5.71	127.93	120.28
1	D	60	ASP	C-N-CA	5.71	127.93	120.28
2	B	67	PHE	CA-CB-CG	5.66	119.46	113.80
1	D	203	SER	CA-C-N	-5.63	113.96	119.76
1	D	203	SER	C-N-CA	-5.63	113.96	119.76
1	D	158	ASN	N-CA-CB	-5.61	103.40	111.54
1	A	3	VAL	N-CA-C	5.60	116.80	108.23
2	E	150	ASN	O-C-N	5.56	129.68	122.40
1	D	42	GLN	CA-C-N	5.54	129.07	120.60
1	D	42	GLN	C-N-CA	5.54	129.07	120.60
2	B	96	ASP	CA-CB-CG	5.45	118.05	112.60
2	E	28	THR	CA-C-N	5.44	127.83	120.38
2	E	28	THR	C-N-CA	5.44	127.83	120.38
1	D	141	PRO	CA-C-N	5.42	128.29	120.38
1	D	141	PRO	C-N-CA	5.42	128.29	120.38
2	E	207	GLU	CA-C-N	-5.40	113.09	119.84
2	E	207	GLU	C-N-CA	-5.40	113.09	119.84
1	D	43	SER	N-CA-C	5.32	117.23	109.84
2	B	94	SER	N-CA-C	-5.29	106.41	112.92
2	B	139	ASP	N-CA-C	5.18	118.39	111.24
2	E	52	ASN	CA-CB-CG	5.07	117.67	112.60
2	B	186	THR	CA-C-N	5.06	127.95	120.82
2	B	186	THR	C-N-CA	5.06	127.95	120.82
1	D	204	PRO	N-CA-C	5.01	118.96	111.14

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	1686	0	1649	19	0
1	D	1677	0	1643	50	0
2	B	1525	0	1502	9	0
2	E	1528	0	1510	30	0
3	C	85	0	82	1	0
3	F	75	0	74	1	0
4	A	76	0	0	0	0
4	B	66	0	0	0	0
4	C	3	0	0	0	0
4	D	56	0	0	2	0
4	E	75	0	0	0	0
4	F	2	0	0	0	0
All	All	6854	0	6460	106	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 8.

All (106) 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:D:147:GLN:OE1	1:D:154:LEU:HD11	1.64	0.98
2:E:190:ILE:HG12	2:E:205:LYS:HD2	1.43	0.96
2:E:118:PRO:HB3	2:E:206:VAL:HG22	1.52	0.91
1:A:36:PHE:HE2	1:A:89:SER:OG	1.57	0.87
1:A:36:PHE:HE2	1:A:89:SER:HG	0.89	0.86
1:D:15:LEU:HD21	1:D:106:ILE:HD13	1.57	0.85
1:D:1:ASP:OD1	1:D:95:PRO:CG	2.24	0.85
2:B:135:CYS:HG	2:B:191:CYS:HG	0.95	0.84
1:A:16:GLY:HA2	1:A:77:ARG:HG3	1.61	0.82
2:E:118:PRO:CB	2:E:206:VAL:HG22	2.10	0.82
1:D:162:SER:OG	2:E:162:PRO:HD2	1.80	0.81
2:E:135:CYS:HG	2:E:191:CYS:HG	0.79	0.78
1:D:55:PHE:HE1	3:F:17:LEU:HD12	1.52	0.75
1:D:1:ASP:OD1	1:D:95:PRO:HG2	1.86	0.74
2:E:149:TRP:HB3	2:E:154:LEU:HD23	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:TYR:CD1	1:D:55:PHE:HD1	2.04	0.74
2:B:70:SER:OG	2:B:79:TYR:HB2	1.86	0.74
1:D:189:HIS:O	1:D:211:ARG:HD3	1.88	0.74
1:D:15:LEU:CD2	1:D:106:ILE:HD13	2.20	0.71
2:E:208:PRO:O	2:E:209:LYS:HB2	1.91	0.71
2:E:190:ILE:CG1	2:E:205:LYS:HD2	2.19	0.69
2:E:118:PRO:HB3	2:E:206:VAL:CG2	2.22	0.69
2:E:150:ASN:ND2	2:E:154:LEU:HD22	2.08	0.69
1:D:49:TYR:CE1	1:D:55:PHE:HD1	2.10	0.69
1:D:34:HIS:ND1	1:D:49:TYR:O	2.28	0.67
2:E:52:ASN:HD21	2:E:55:SER:HB2	1.64	0.63
1:D:32:TYR:CE1	1:D:50:LYS:HE2	2.33	0.62
1:D:147:GLN:OE1	1:D:154:LEU:CD1	2.45	0.61
1:D:49:TYR:CD1	1:D:55:PHE:CD1	2.88	0.60
2:E:190:ILE:HG12	2:E:205:LYS:CD	2.24	0.60
1:A:46:LEU:HD21	1:A:49:TYR:HB3	1.84	0.60
1:D:46:LEU:HD21	1:D:49:TYR:HB3	1.82	0.60
1:A:33:LEU:HD13	1:A:71:PHE:CD2	2.37	0.59
1:D:32:TYR:HB2	1:D:92:THR:HG23	1.84	0.59
1:D:169:LYS:HD2	1:D:169:LYS:N	2.18	0.58
1:D:90:GLN:NE2	1:D:97:THR:OG1	2.36	0.58
2:E:150:ASN:HB2	2:E:154:LEU:HB2	1.86	0.58
1:A:33:LEU:HD13	1:A:71:PHE:CE2	2.38	0.58
1:D:106:ILE:HD11	1:D:171:SER:CB	2.34	0.57
1:D:33:LEU:HD22	1:D:71:PHE:CD1	2.39	0.57
2:B:12:VAL:HG11	2:B:82(C):LEU:HD13	1.87	0.57
1:A:24:ARG:HG2	1:A:70:ASP:OD1	2.05	0.57
1:D:1:ASP:OD1	1:D:95:PRO:HG3	2.05	0.56
2:E:118:PRO:HD3	2:E:204:LYS:HE2	1.86	0.55
2:E:137:VAL:HG11	2:E:145:VAL:HG11	1.89	0.55
1:D:143:GLU:H	1:D:143:GLU:CD	2.14	0.54
1:D:33:LEU:HD22	1:D:71:PHE:CG	2.43	0.54
1:D:79:GLU:HB3	1:D:81:GLU:HG2	1.88	0.54
2:E:82:MET:HE2	2:E:82(C):LEU:HD21	1.89	0.54
1:D:145:LYS:HB3	1:D:197:THR:HB	1.90	0.53
2:E:179:VAL:HG12	2:E:180:PRO:O	2.08	0.53
1:D:27(E):SER:C	1:D:29:GLY:H	2.16	0.53
1:A:23:CYS:HG	1:A:88:CYS:HG	1.53	0.52
1:D:32:TYR:HB2	1:D:92:THR:CG2	2.40	0.51
2:E:78:LEU:HD23	2:E:92:CYS:SG	2.52	0.50
2:B:70:SER:HG	2:B:79:TYR:HB2	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD22	1:A:71:PHE:CD1	2.47	0.49
1:A:108:ARG:HD3	1:A:109:THR:O	2.12	0.49
1:A:83:VAL:HG21	1:A:166:GLN:HB3	1.95	0.49
1:D:27(A):SER:OG	1:D:27(C):ILE:HG22	2.13	0.49
1:D:203:SER:OG	1:D:204:PRO:CD	2.61	0.48
1:D:28:ASP:HB2	4:D:338:HOH:O	2.11	0.48
2:E:12:VAL:HG11	2:E:82(C):LEU:HD13	1.95	0.48
1:D:187:GLU:OE1	1:D:211:ARG:NH2	2.47	0.48
1:A:90:GLN:OE1	1:A:92:THR:N	2.46	0.47
1:D:79:GLU:OE2	1:D:81:GLU:OE1	2.32	0.47
1:D:27(B):LEU:O	1:D:92:THR:HG21	2.15	0.47
1:D:106:ILE:HD11	1:D:171:SER:OG	2.14	0.47
1:A:47:LEU:HA	1:A:58:VAL:HG21	1.96	0.47
1:D:32:TYR:HE1	1:D:50:LYS:HE2	1.80	0.46
1:D:141:PRO:HB2	1:D:143:GLU:OE1	2.15	0.46
2:E:118:PRO:HB2	2:E:206:VAL:HG22	1.95	0.46
1:A:37:LEU:HB2	1:A:47:LEU:HD11	1.97	0.46
1:D:27(E):SER:C	1:D:29:GLY:N	2.73	0.46
2:E:87:THR:HG23	2:E:105:THR:HA	1.97	0.46
1:D:27(B):LEU:HD22	1:D:90:GLN:HG3	1.97	0.46
1:D:79:GLU:OE2	1:D:81:GLU:CD	2.59	0.45
1:A:61:ARG:HB2	1:A:76:SER:HB2	1.98	0.45
1:A:23:CYS:SG	1:A:88:CYS:SG	3.02	0.45
2:E:149:TRP:O	2:E:154:LEU:HB3	2.15	0.45
2:B:82:MET:HE2	2:B:82(C):LEU:HD21	1.99	0.45
1:D:27(D):TYR:CG	1:D:27(E):SER:N	2.85	0.45
3:C:18:VAL:HG13	3:C:23:ASP:HB2	1.98	0.44
1:D:54:ARG:HD2	4:D:319:HOH:O	2.18	0.43
2:E:121:PRO:HG2	2:E:208:PRO:HB3	2.01	0.43
1:A:63:SER:HB3	1:A:74:LYS:HG3	1.99	0.43
1:D:145:LYS:HE2	1:D:147:GLN:HE21	1.83	0.42
1:D:95:PRO:HB3	2:E:58:TYR:CE1	2.55	0.42
2:E:149:TRP:C	2:E:154:LEU:HB3	2.44	0.42
2:B:135:CYS:SG	2:B:206:VAL:HG21	2.60	0.42
1:D:138:ASN:C	1:D:172:THR:HB	2.44	0.42
1:D:143:GLU:CD	1:D:143:GLU:N	2.77	0.41
2:E:11:LEU:HD22	2:E:142:PRO:HG3	2.02	0.41
1:A:32:TYR:CE2	1:A:50:LYS:HD3	2.56	0.41
1:D:12:PRO:HA	1:D:105:GLU:O	2.20	0.41
2:E:114:PRO:HB3	2:E:140:TYR:HB3	2.02	0.41
1:A:96:TRP:HZ3	2:B:35:SER:OG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ALA:HA	2:B:173:LEU:HB3	2.03	0.41
2:E:121:PRO:HD2	2:E:208:PRO:HA	2.02	0.41
1:D:21:ILE:HG12	1:D:102:THR:HG21	2.03	0.41
1:D:63:SER:HB3	1:D:74:LYS:HG3	2.03	0.41
2:E:189:TYR:O	2:E:205:LYS:HE3	2.20	0.40
2:E:142:PRO:HD2	2:E:197:PRO:HB2	2.03	0.40
1:D:66:GLY:HA3	1:D:71:PHE:CD1	2.57	0.40
2:B:135:CYS:SG	2:B:206:VAL:CG2	3.09	0.40
1:D:5:THR:HB	1:D:24:ARG:HB3	2.04	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	A	216/219 (99%)	207 (96%)	9 (4%)	0	100	100
1	D	215/219 (98%)	203 (94%)	12 (6%)	0	100	100
2	B	202/223 (91%)	193 (96%)	9 (4%)	0	100	100
2	E	202/223 (91%)	192 (95%)	10 (5%)	0	100	100
3	C	9/17 (53%)	8 (89%)	1 (11%)	0	100	100
3	F	7/17 (41%)	7 (100%)	0	0	100	100
All	All	851/918 (93%)	810 (95%)	41 (5%)	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	194/195 (100%)	186 (96%)	8 (4%)	27	44
1	D	193/195 (99%)	186 (96%)	7 (4%)	31	50
2	B	172/188 (92%)	171 (99%)	1 (1%)	78	88
2	E	172/188 (92%)	165 (96%)	7 (4%)	27	44
3	C	9/15 (60%)	9 (100%)	0	100	100
3	F	8/15 (53%)	7 (88%)	1 (12%)	4	6
All	All	748/796 (94%)	724 (97%)	24 (3%)	34	54

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	2	VAL
1	A	24	ARG
1	A	34	HIS
1	A	61	ARG
1	A	108	ARG
1	A	145	LYS
1	A	163	VAL
2	B	75	LYS
1	D	54	ARG
1	D	77	ARG
1	D	90	GLN
1	D	103	LYS
1	D	132	VAL
1	D	169	LYS
1	D	195	GLU
2	E	28	THR
2	E	143	GLU
2	E	145	VAL
2	E	187	GLN
2	E	205	LYS
2	E	206	VAL
2	E	207	GLU
3	F	24	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	B	166	GLN
2	B	194	ASN
1	D	53	ASN
1	D	90	GLN
1	D	124	GLN
1	D	210	ASN
2	E	50	GLN
2	E	76	ASN
2	E	192	ASN

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	A	218/219 (99%)	1.03	21 (9%) 13 10	22, 35, 52, 76	0
1	D	217/219 (99%)	1.71	83 (38%) 1 0	22, 50, 81, 103	0
2	B	206/223 (92%)	0.74	19 (9%) 14 11	12, 27, 52, 76	0
2	E	206/223 (92%)	1.10	38 (18%) 3 3	14, 30, 70, 120	0
3	C	11/17 (64%)	1.65	4 (36%) 1 0	33, 38, 60, 78	0
3	F	9/17 (52%)	1.74	2 (22%) 2 2	40, 44, 58, 86	0
All	All	867/918 (94%)	1.16	167 (19%) 3 2	12, 36, 67, 120	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	206	VAL	6.6
2	E	121	PRO	5.0
2	E	182	SER	4.8
2	B	123	SER	4.8
2	E	186	THR	4.7
2	E	135	CYS	4.7
2	E	183	SER	4.6
2	E	209	LYS	4.4
1	D	67	SER	4.4
2	E	26	GLY	4.3
2	E	184	LEU	4.1
2	E	208	PRO	4.0
1	D	134	CYS	3.9
1	D	183	LYS	3.9
2	E	192	ASN	3.9
2	E	122	SER	3.7
3	F	24	VAL	3.7
1	D	32	TYR	3.6
2	E	188	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	212	GLY	3.6
1	D	49	TYR	3.5
1	D	80	ALA	3.5
1	D	30	ASN	3.5
1	D	78	VAL	3.5
2	B	185	GLY	3.4
2	B	186	THR	3.4
2	E	190	ILE	3.4
1	D	40	PRO	3.3
2	E	185	GLY	3.3
1	D	27(E)	SER	3.3
1	D	186	TYR	3.3
1	D	177	SER	3.3
1	D	150	VAL	3.2
2	E	205	LYS	3.2
2	E	129	GLY	3.2
1	D	56	SER	3.2
1	A	176	SER	3.2
1	D	77	ARG	3.1
1	D	190	LYS	3.1
1	D	58	VAL	3.1
2	E	187	GLN	3.1
1	D	153	ALA	3.1
1	D	27	GLN	3.0
1	D	209	PHE	3.0
1	D	26	SER	3.0
3	F	16	LYS	3.0
1	D	105	GLU	3.0
1	A	125	LEU	3.0
2	B	26	GLY	3.0
1	A	56	SER	3.0
1	D	23	CYS	3.0
2	B	135	CYS	2.9
1	D	110	VAL	2.9
1	D	121	SER	2.9
2	E	57	THR	2.9
1	A	32	TYR	2.9
1	A	200	GLY	2.9
1	D	176	SER	2.9
2	B	122	SER	2.9
1	A	27(C)	ILE	2.9
1	D	111	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	189	TYR	2.8
1	D	25	SER	2.8
2	B	182	SER	2.8
3	C	24	VAL	2.8
1	A	134	CYS	2.8
1	D	31	ALA	2.8
2	B	3	GLN	2.8
2	B	9	GLY	2.8
3	C	25	GLY	2.8
1	D	15	LEU	2.8
2	E	175	SER	2.7
1	D	50	LYS	2.7
3	C	26	SER	2.7
1	A	31	ALA	2.7
1	D	163	VAL	2.7
1	A	57	GLY	2.7
2	E	130	THR	2.7
1	A	213	GLU	2.6
1	D	210	ASN	2.6
1	D	187	GLU	2.6
2	E	131	ALA	2.6
1	D	122	ASP	2.6
2	B	136	LEU	2.6
1	D	14	THR	2.6
1	D	184	ALA	2.6
2	E	120	ALA	2.6
1	A	70	ASP	2.6
2	B	57	THR	2.6
2	E	178	THR	2.6
2	E	207	GLU	2.5
1	D	144	ALA	2.5
1	D	112	ALA	2.5
1	D	202	SER	2.5
2	E	22	CYS	2.5
2	E	191	CYS	2.5
1	D	70	ASP	2.5
1	D	135	LEU	2.5
1	D	206	THR	2.5
2	B	188	THR	2.5
1	D	125	LEU	2.5
1	D	131	SER	2.5
2	E	150	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	28	THR	2.4
2	B	55	SER	2.4
1	A	187	GLU	2.4
1	D	106	ILE	2.4
1	D	146	VAL	2.4
1	D	109	THR	2.4
2	E	181	SER	2.4
1	D	205	VAL	2.4
1	A	111	ALA	2.4
1	D	120	PRO	2.4
1	D	171	SER	2.4
1	D	182	SER	2.4
2	B	183	SER	2.3
1	D	61	ARG	2.3
1	D	42	GLN	2.3
1	A	66	GLY	2.3
3	C	17	LEU	2.3
2	E	27	PHE	2.3
1	D	123	GLU	2.3
2	E	180	PRO	2.3
1	D	148	TRP	2.3
2	E	95	GLY	2.3
2	E	177	VAL	2.3
1	D	27(A)	SER	2.3
1	D	27(C)	ILE	2.3
1	A	55	PHE	2.3
2	B	29	PHE	2.2
1	D	211	ARG	2.2
2	E	92	CYS	2.2
1	A	109	THR	2.2
1	A	89	SER	2.2
1	D	1	ASP	2.2
2	B	27	PHE	2.2
1	A	3	VAL	2.2
1	D	133	VAL	2.2
1	D	191	VAL	2.2
1	D	107	LYS	2.2
1	D	197	THR	2.2
1	D	22	SER	2.2
1	D	43	SER	2.2
1	D	57	GLY	2.1
1	A	67	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	108	ARG	2.1
1	D	114	SER	2.1
1	D	83	VAL	2.1
1	D	160	GLN	2.1
2	B	187	GLN	2.1
1	D	76	SER	2.1
1	D	162	SER	2.1
2	E	179	VAL	2.1
1	D	154	LEU	2.1
1	D	199	GLN	2.1
1	D	142	ARG	2.1
1	D	129	THR	2.1
1	D	164	THR	2.1
1	A	76	SER	2.1
1	D	194	CYS	2.1
1	D	132	VAL	2.0
2	E	153	ALA	2.0
1	A	106	ILE	2.0
1	D	60	ASP	2.0
1	D	118	PHE	2.0
2	E	204	LYS	2.0
2	B	180	PRO	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.