Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:27 PM GMT

PDB ID	:	4XXD
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

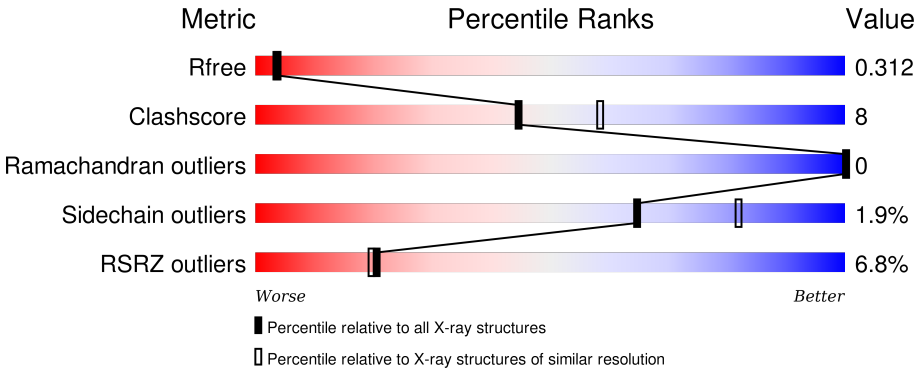
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	3%, 85%, 13%
1	D	219	14%, 74%, 21%
2	B	223	%, 87%, 5%, 8%
2	E	223	8%, 75%, 16%, 8%
3	C	17	12%, 53%, 12%, 35%

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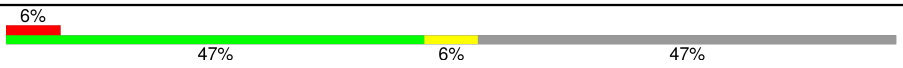
Mol	Chain	Length	Quality of chain
3	F	17	

2 Entry composition

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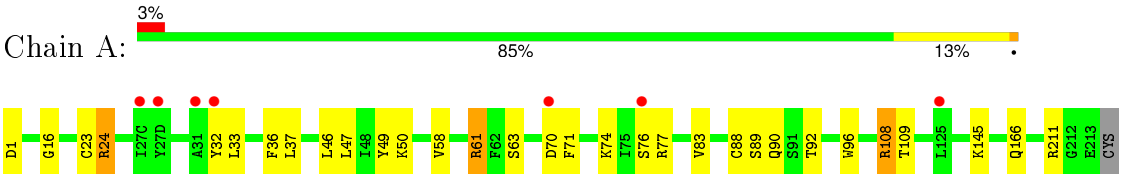
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	75	Total O 75 75	0	0
4	F	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

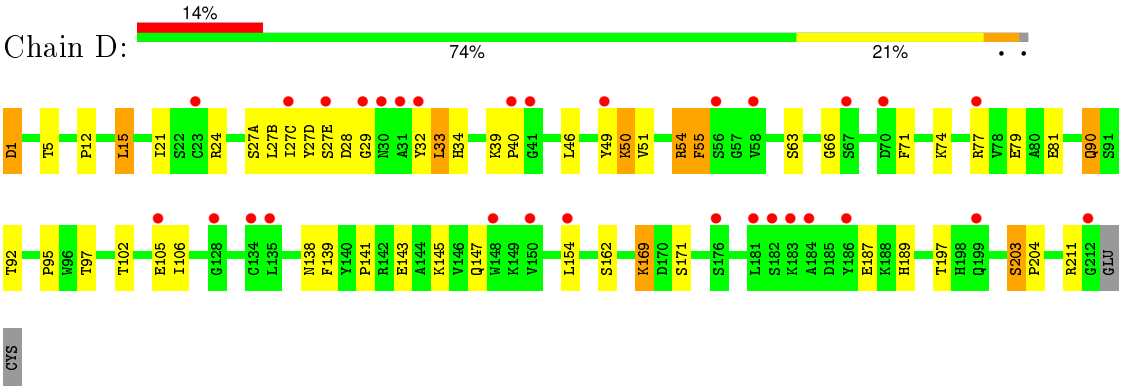
- Molecule 1: Fab Light Chain

Chain A:



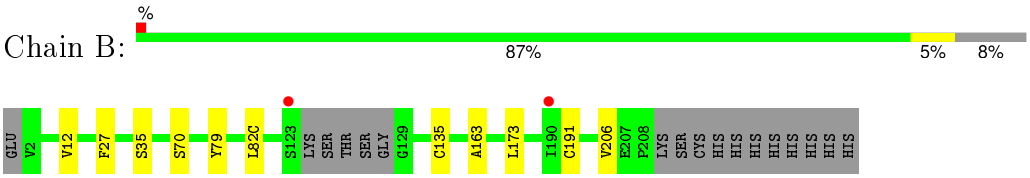
- Molecule 1: Fab Light Chain

Chain D:



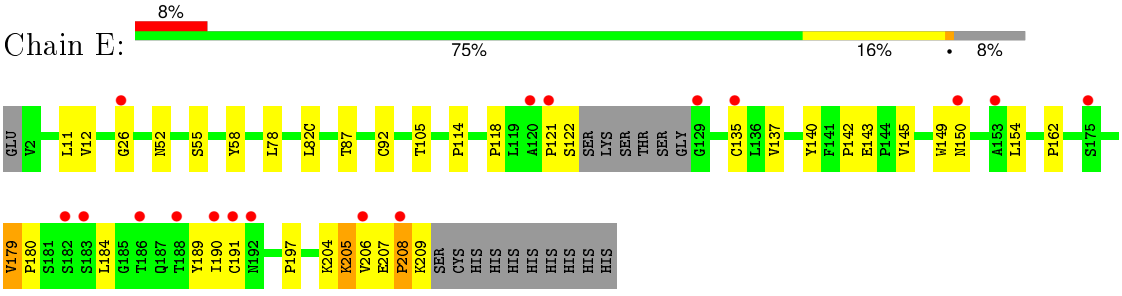
- Molecule 2: Fab Heavy Chain

Chain B:



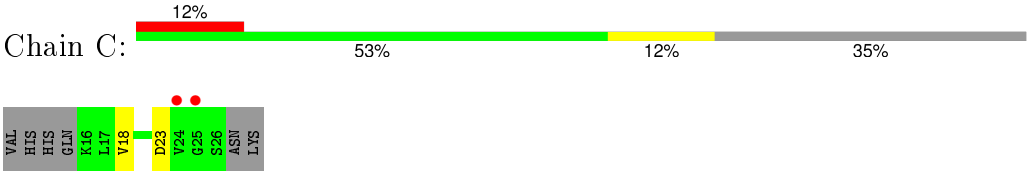
- Molecule 2: Fab Heavy Chain

Chain E:



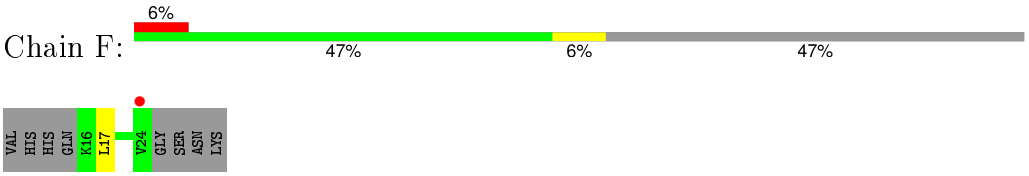
• Molecule 3: Amyloid-beta fragment

Chain C:



• Molecule 3: Amyloid-beta fragment

Chain F:



4 Data and refinement statistics (i)

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 46.57 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.56-2.41) 86.5 (46.57-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.249 , 0.290 0.265 , 0.312	Depositor DCC
R_{free} test set	1796 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 35909 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.51	0/1725	0.71	2/2343 (0.1%)
1	D	0.74	1/1716 (0.1%)	0.87	10/2331 (0.4%)
2	B	0.46	0/1559	0.73	2/2125 (0.1%)
2	E	0.48	1/1562 (0.1%)	0.79	4/2128 (0.2%)
3	C	0.40	0/86	0.68	0/114
3	F	0.43	0/76	0.70	0/101
All	All	0.56	2/6724 (0.0%)	0.78	18/9142 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	40	PRO	N-CD	9.94	1.61	1.47
2	E	208	PRO	N-CD	5.52	1.55	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	184	LEU	CB-CA-C	9.99	129.19	110.20
2	B	27	PHE	N-CA-CB	-8.07	96.07	110.60
1	A	211	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	D	39	LYS	CB-CA-C	7.71	125.82	110.40
1	D	138	ASN	N-CA-C	7.14	130.28	111.00
2	B	27	PHE	N-CA-C	6.97	129.83	111.00
1	D	40	PRO	CA-N-CD	-6.83	101.94	111.50
1	D	15	LEU	CB-CG-CD2	6.14	121.44	111.00
1	A	211	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	D	50	LYS	CB-CA-C	-6.01	98.38	110.40
1	D	203	SER	C-N-CD	5.78	140.54	128.40
2	E	26	GLY	N-CA-C	5.68	127.30	113.10
1	D	51	VAL	N-CA-CB	5.65	123.92	111.50
1	D	139	PHE	N-CA-CB	-5.64	100.45	110.60
2	E	207	GLU	C-N-CD	5.37	139.67	128.40
1	D	33	LEU	CB-CG-CD1	5.36	120.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	179	VAL	CB-CA-C	-5.36	101.22	111.40
1	D	50	LYS	N-CA-C	5.08	124.72	111.00

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	48	0
2	B	1525	0	1502	8	0
2	E	1528	0	1510	28	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	101	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 (101) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:23:CYS:HG	1:A:88:CYS:HG	1.43	0.66
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:D:46:LEU:HD21	1:D:49:TYR:HB3	1.82	0.60
1:A:46:LEU:HD21	1:A:49:TYR:HB3	1.84	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:33:LEU:HD22	1:D:71:PHE:CG	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:GLU:HB3	1:D:81:GLU:HG2	1.88	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: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
1:D:143:GLU:CD	1:D:143:GLU:H	2.14	0.50
2:B:70:SER:HG	2:B:79:TYR:HB2	1.73	0.49
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(E):SER:C	1:D:29:GLY:H	2.16	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
2:E:12:VAL:HG11	2:E:82(C):LEU:HD13	1.95	0.48
1:D:28:ASP:HB2	4:D:338:HOH:O	2.11	0.48
1:D:187:GLU:OE1	1:D:211:ARG:NH2	2.47	0.48
1:D:79:GLU:OE2	1:D:81:GLU:OE1	2.32	0.47
1:A:90:GLN:OE1	1:A:92:THR:N	2.46	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
2:E:118:PRO:HB2	2:E:206:VAL:HG22	1.95	0.46
1:D:141:PRO:HB2	1:D:143:GLU:OE1	2.15	0.46
1:A:37:LEU:HB2	1:A:47:LEU:HD11	1.97	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: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
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:B:135:CYS:SG	2:B:206:VAL:HG21	2.60	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27(E):SER:C	1:D:29:GLY:N	2.73	0.41
2:E:114:PRO:HB3	2:E:140:TYR:HB3	2.02	0.41
2:E:121:PRO:HD2	2:E:208:PRO:HA	2.02	0.41
2:B:163:ALA:HA	2:B:173:LEU:HB3	2.03	0.41
1:A:96:TRP:HZ3	2:B:35:SER:OG	2.03	0.41
1:D:79:GLU:OE2	1:D:81:GLU:CD	2.59	0.41
1:D:63:SER:HB3	1:D:74:LYS:HG3	2.03	0.41
1:D:21:ILE:HG12	1:D:102:THR:HG21	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%)	189 (97%)	5 (3%)	54 74
1	D	193/195 (99%)	187 (97%)	6 (3%)	47 68
2	B	172/188 (92%)	172 (100%)	0	100 100
2	E	172/188 (92%)	169 (98%)	3 (2%)	68 84
3	C	9/15 (60%)	9 (100%)	0	100 100
3	F	8/15 (53%)	8 (100%)	0	100 100
All	All	748/796 (94%)	734 (98%)	14 (2%)	65 82

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

Mol	Chain	Res	Type
1	A	1	ASP
1	A	24	ARG
1	A	61	ARG
1	A	108	ARG
1	A	145	LYS
1	D	1	ASP
1	D	54	ARG
1	D	55	PHE
1	D	77	ARG
1	D	90	GLN
1	D	169	LYS
2	E	122	SER
2	E	143	GLU
2	E	205	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	ASN
1	D	90	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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%)	0.43	7 (3%) 51 50	22, 35, 52, 76	0
1	D	217/219 (99%)	0.95	30 (13%) 4 4	22, 50, 81, 103	0
2	B	206/223 (92%)	0.23	2 (0%) 84 83	12, 27, 52, 76	0
2	E	206/223 (92%)	0.50	17 (8%) 14 13	14, 30, 70, 120	0
3	C	11/17 (64%)	1.27	2 (18%) 2 1	33, 38, 60, 78	0
3	F	9/17 (52%)	1.18	1 (11%) 7 7	40, 44, 58, 86	0
All	All	867/918 (94%)	0.55	59 (6%) 20 20	12, 36, 67, 120	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	27(E)	SER	6.8
2	E	206	VAL	6.1
1	D	183	LYS	5.7
1	D	67	SER	5.2
3	F	24	VAL	4.5
2	E	186	THR	4.4
1	D	184	ALA	4.1
3	C	24	VAL	4.0
1	D	154	LEU	4.0
1	D	29	GLY	3.7
2	E	208	PRO	3.5
2	E	121	PRO	3.4
2	E	182	SER	3.3
1	D	40	PRO	3.3
2	B	123	SER	3.2
2	E	183	SER	3.2
1	D	30	ASN	3.2
2	E	135	CYS	3.2
1	D	31	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	25	GLY	3.0
2	E	129	GLY	2.9
1	D	176	SER	2.9
1	A	70	ASP	2.9
1	D	49	TYR	2.8
1	D	182	SER	2.8
1	D	27(C)	ILE	2.7
2	E	190	ILE	2.7
1	D	150	VAL	2.6
1	A	32	TYR	2.6
2	E	188	THR	2.6
1	A	27(D)	TYR	2.6
1	D	32	TYR	2.5
1	D	134	CYS	2.5
2	E	26	GLY	2.5
1	D	105	GLU	2.5
1	D	186	TYR	2.4
1	D	135	LEU	2.4
2	B	190	ILE	2.4
1	D	23	CYS	2.4
1	D	41	GLY	2.4
1	D	58	VAL	2.4
2	E	153	ALA	2.3
1	D	148	TRP	2.3
1	A	31	ALA	2.3
1	D	212	GLY	2.2
2	E	120	ALA	2.2
1	D	181	LEU	2.2
1	D	128	GLY	2.2
1	A	76	SER	2.2
1	D	199	GLN	2.2
2	E	150	ASN	2.2
1	A	27(C)	ILE	2.1
1	D	70	ASP	2.1
2	E	191	CYS	2.1
1	A	125	LEU	2.1
1	D	77	ARG	2.0
2	E	192	ASN	2.0
2	E	175	SER	2.0
1	D	56	SER	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.