Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 09:12 PM EDT

PDB ID	:	6S3D
Title	:	Structure of D25 Fab in complex with scaffold S0_2.126
Authors	:	Cramer, J.T.; Krey, T.
Deposited on	:	2019-06-25
Resolution	:	3.00 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:

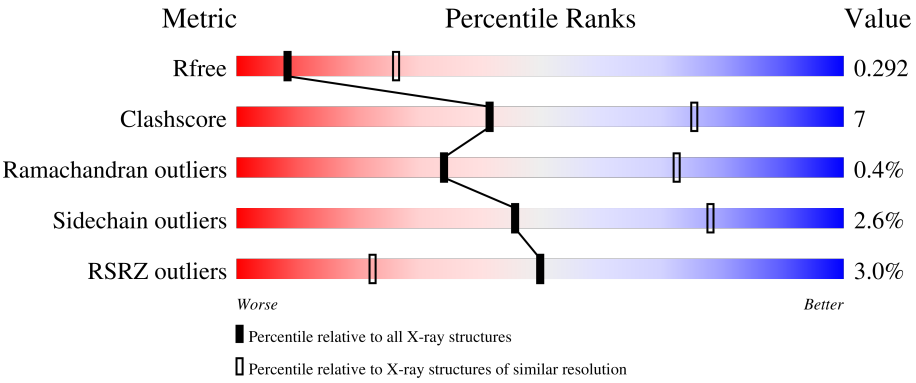
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	241	5% 75% 12% • 12%
1	C	241	2% 77% 12% 11%
1	E	241	3% 73% 16% 11%
1	H	241	4% 71% 16% • 12%
2	B	225	3% 79% 14% • 7%

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Mol	Chain	Length	Quality of chain
2	D	225	3% 75% 16% 8%
2	F	225	% 76% 15% 8%
2	L	225	3% 77% 16% 6%
3	M	71	% 62% 21% 17%
3	N	71	% 62% 20% 18%
3	O	71	% 62% 17% 17%
3	P	71	56% 25% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14439 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 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1572	1002	259	304	7			
1	C	215	Total	C	N	O	S	0	0	0
			1601	1020	265	309	7			
1	E	215	Total	C	N	O	S	0	0	0
			1590	1012	264	307	7			
1	H	212	Total	C	N	O	S	0	0	0
			1581	1006	261	307	7			

- Molecule 2 is a protein called Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1580	991	260	324	5			
2	D	206	Total	C	N	O	S	0	0	0
			1570	986	260	319	5			
2	F	206	Total	C	N	O	S	0	0	0
			1553	972	256	320	5			
2	L	211	Total	C	N	O	S	0	0	0
			1585	992	261	327	5			

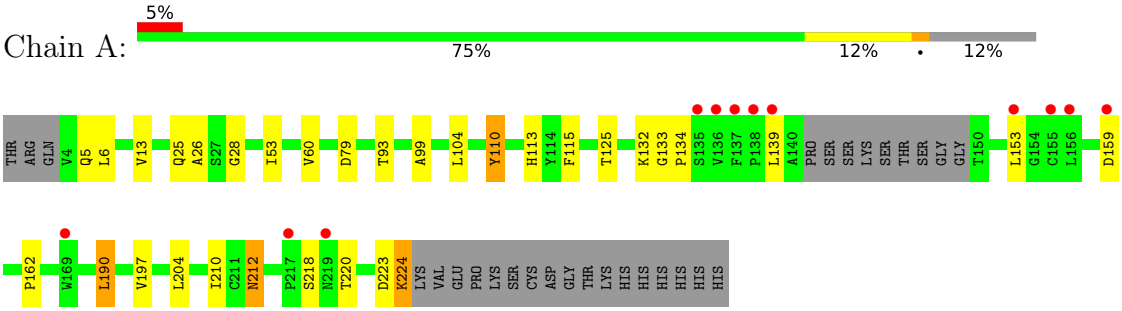
- Molecule 3 is a protein called S0_2.126.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	59	Total	C	N	O	S	0	0	0
			444	277	77	85	5			
3	N	58	Total	C	N	O	S	0	0	0
			456	284	80	87	5			
3	O	59	Total	C	N	O	S	0	0	0
			452	280	79	88	5			
3	P	58	Total	C	N	O	S	0	0	0
			455	282	82	87	4			

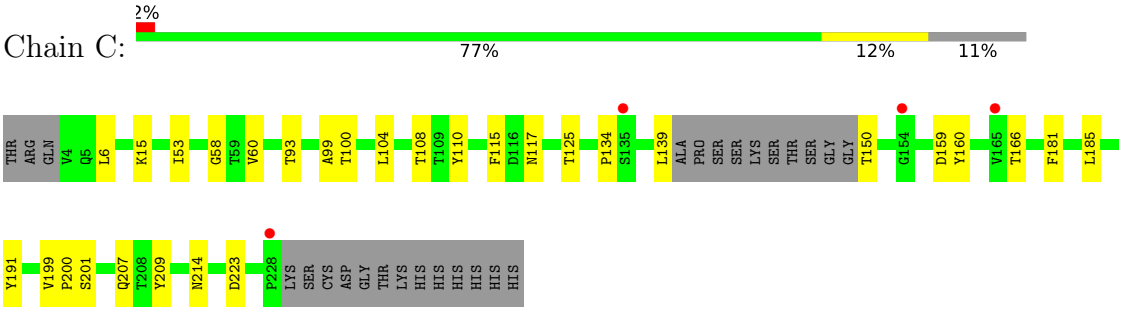
3 Residue-property plots (i)

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.

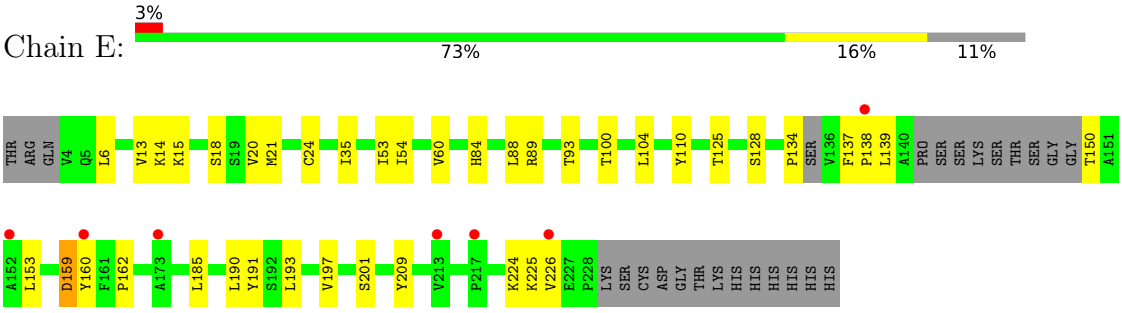
• Molecule 1: Heavy Chain



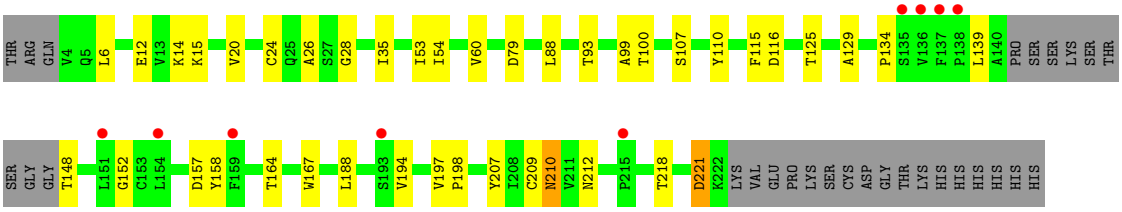
• Molecule 1: Heavy Chain



• Molecule 1: Heavy Chain

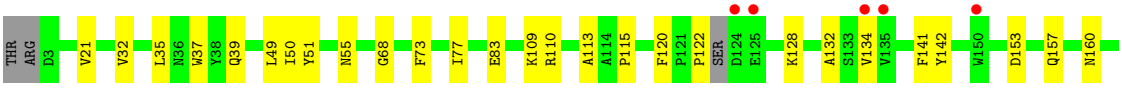


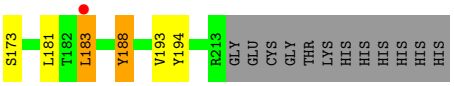
• Molecule 1: Heavy Chain



• Molecule 2: Light Chain

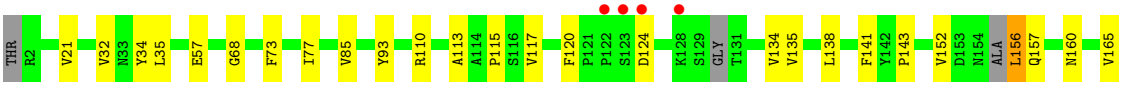
Chain B:

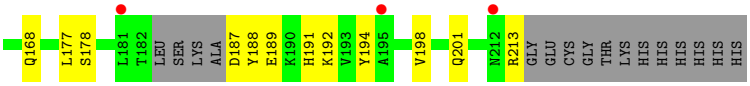




• Molecule 2: Light Chain

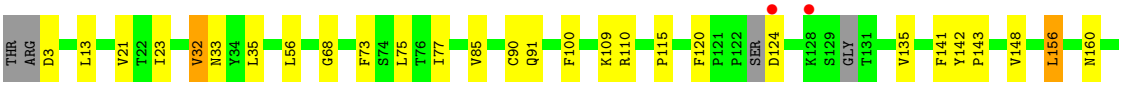
Chain D:

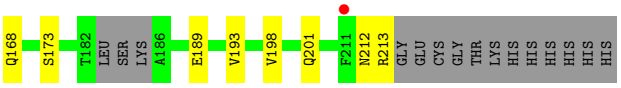




• Molecule 2: Light Chain

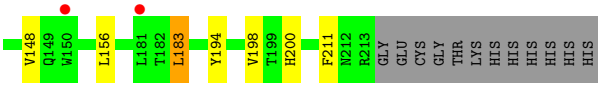
Chain F:





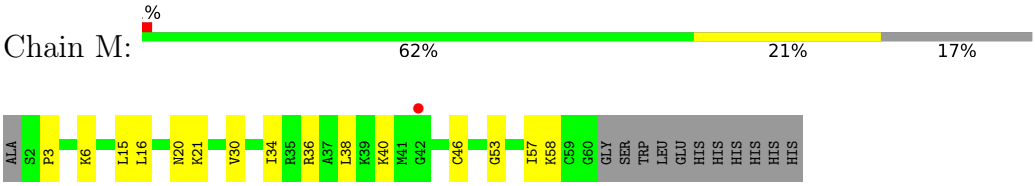
• Molecule 2: Light Chain

Chain L:



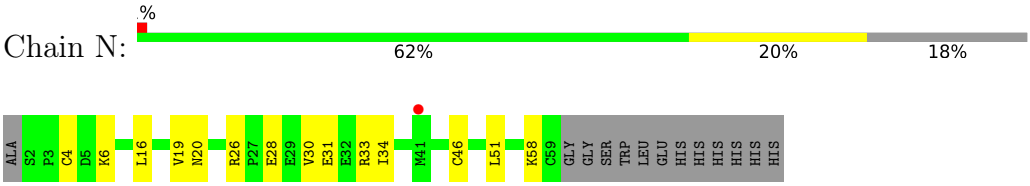
• Molecule 3: S0_2.126

Chain M:



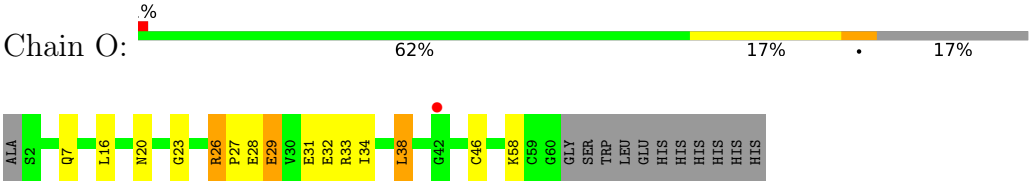
• Molecule 3: S0_2.126

Chain N:



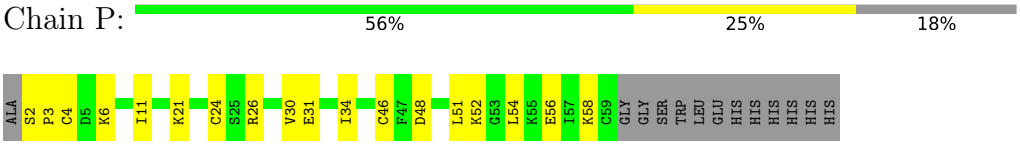
• Molecule 3: S0_2.126

Chain O:



• Molecule 3: S0_2.126

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.27Å 126.98Å 156.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 3.00 49.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.09-3.00) 99.7 (49.09-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.269 , 0.292 0.270 , 0.292	Depositor DCC
R_{free} test set	2542 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	73.4	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14439	wwPDB-VP
Average B, all atoms (Å^2)	100.0	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 88.81 % 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 4.2895e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.28	0/1612	0.55	0/2211
1	C	0.27	0/1642	0.53	0/2250
1	E	0.33	0/1629	0.58	0/2232
1	H	0.26	0/1621	0.53	0/2221
2	B	0.28	0/1612	0.51	0/2199
2	D	0.30	0/1600	0.53	0/2175
2	F	0.28	0/1583	0.51	0/2158
2	L	0.28	0/1617	0.50	0/2206
3	M	0.36	0/447	0.53	0/596
3	N	0.33	0/460	0.51	0/612
3	O	0.41	0/456	0.70	0/609
3	P	0.30	0/459	0.55	0/612
All	All	0.30	0/14738	0.54	0/20081

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

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	1572	0	1525	21	0
1	C	1601	0	1562	15	0
1	E	1590	0	1539	23	0
1	H	1581	0	1546	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1580	0	1503	19	0
2	D	1570	0	1502	28	0
2	F	1553	0	1454	22	0
2	L	1585	0	1506	24	0
3	M	444	0	440	11	0
3	N	456	0	470	7	0
3	O	452	0	451	11	0
3	P	455	0	463	9	0
All	All	14439	0	13961	199	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 7.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:26:ARG:O	3:O:29:GLU:HB2	1.54	1.08
1:E:159:ASP:HB3	1:E:190:LEU:HD22	1.55	0.87
3:O:28:GLU:HA	3:O:31:GLU:HG3	1.62	0.79
1:E:14:LYS:HG3	1:E:20:VAL:HG12	1.68	0.74
3:O:26:ARG:CZ	3:O:28:GLU:HB2	2.18	0.74
1:A:13:VAL:HG22	1:A:162:PRO:HG3	1.71	0.71
1:H:194:VAL:HG21	2:L:137:LEU:HD11	1.73	0.71
3:N:19:VAL:HG22	3:N:33:ARG:HE	1.56	0.70
1:E:13:VAL:HG22	1:E:162:PRO:HG3	1.75	0.69
1:E:150:THR:N	1:E:201:SER:HG	1.90	0.69
1:A:104:LEU:HD12	3:N:58:LYS:HB2	1.73	0.69
1:C:150:THR:N	1:C:201:SER:HG	1.92	0.67
3:O:34:ILE:O	3:O:38:LEU:HD22	1.94	0.67
3:M:16:LEU:O	3:M:20:ASN:ND2	2.26	0.67
2:D:189:GLU:HA	2:D:213:ARG:HH12	1.61	0.66
1:C:93:THR:HG23	1:C:125:THR:HA	1.77	0.65
1:H:15:LYS:NZ	1:H:129:ALA:O	2.29	0.65
1:H:93:THR:HG23	1:H:125:THR:HA	1.78	0.64
2:F:23:ILE:HD11	2:F:75:LEU:HD23	1.81	0.63
2:F:110:ARG:HD2	2:F:173:SER:HB2	1.81	0.63
2:D:152:VAL:HG12	2:D:194:TYR:CD1	2.33	0.63
2:F:68:GLY:HA3	2:F:73:PHE:HA	1.81	0.63
3:O:7:GLN:NE2	3:O:46:CYS:SG	2.72	0.62
2:L:68:GLY:HA3	2:L:73:PHE:HA	1.83	0.61
2:L:115:PRO:HB3	2:L:141:PHE:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:16:LEU:O	3:O:20:ASN:ND2	2.34	0.60
2:F:156:LEU:H	2:F:156:LEU:HD23	1.67	0.60
2:F:21:VAL:HG22	2:F:77:ILE:HB	1.83	0.60
1:H:210:ASN:ND2	1:H:221:ASP:OD1	2.35	0.60
1:H:134:PRO:HB3	1:H:158:TYR:HB3	1.84	0.60
2:B:122:PRO:HD3	2:B:134:VAL:HG22	1.85	0.59
1:E:93:THR:HG23	1:E:125:THR:HA	1.84	0.59
3:M:30:VAL:CG2	3:M:57:ILE:HD11	2.33	0.59
1:A:93:THR:HG23	1:A:125:THR:HA	1.85	0.59
2:B:68:GLY:HA3	2:B:73:PHE:HA	1.86	0.58
1:C:134:PRO:HB3	1:C:160:TYR:HB3	1.86	0.58
2:B:21:VAL:HG22	2:B:77:ILE:HB	1.86	0.57
1:H:53:ILE:HG13	1:H:60:VAL:HG22	1.86	0.57
1:C:199:VAL:HG21	1:C:209:TYR:OH	2.04	0.57
2:F:32:VAL:HG13	2:F:33:ASN:H	1.70	0.57
1:H:139:LEU:HD21	2:L:135:VAL:HG21	1.87	0.57
1:C:150:THR:HG22	1:C:200:PRO:HA	1.86	0.57
2:F:124:ASP:N	2:F:124:ASP:OD1	2.38	0.57
3:M:30:VAL:HG21	3:M:57:ILE:HD11	1.86	0.57
2:B:188:TYR:HA	2:B:194:TYR:OH	2.04	0.56
1:A:6:LEU:HD23	1:A:26:ALA:HB2	1.88	0.56
3:N:16:LEU:O	3:N:20:ASN:ND2	2.36	0.56
2:F:120:PHE:HB2	2:F:135:VAL:HG22	1.87	0.56
1:A:53:ILE:HG13	1:A:60:VAL:HG22	1.88	0.56
2:B:39:GLN:HB2	2:B:49:LEU:HD11	1.86	0.56
1:E:224:LYS:HE3	1:E:225:LYS:H	1.71	0.55
2:D:21:VAL:HG22	2:D:77:ILE:HB	1.87	0.55
1:A:139:LEU:HD22	2:B:120:PHE:HB3	1.88	0.55
2:F:3:ASP:N	2:F:3:ASP:OD1	2.40	0.55
2:D:192:LYS:HA	2:D:213:ARG:HD3	1.89	0.55
2:L:148:VAL:HG22	2:L:198:VAL:HG22	1.88	0.55
3:M:36:ARG:O	3:M:40:LYS:HD3	2.06	0.54
2:L:21:VAL:HG22	2:L:77:ILE:HB	1.88	0.54
2:F:85:VAL:HG11	2:F:168:GLN:HB3	1.89	0.54
3:M:34:ILE:O	3:M:38:LEU:HG	2.07	0.54
3:P:4:CYS:O	3:P:6:LYS:N	2.35	0.54
1:A:5:GLN:O	1:A:26:ALA:HA	2.08	0.53
1:A:212:ASN:ND2	1:A:223:ASP:OD1	2.42	0.53
2:B:157:GLN:HB3	2:B:160:ASN:HD21	1.73	0.53
1:C:104:LEU:HB3	3:M:58:LYS:O	2.08	0.53
1:E:159:ASP:N	1:E:159:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:LEU:HB3	2:F:120:PHE:HB3	1.90	0.52
2:B:160:ASN:OD1	2:B:160:ASN:N	2.43	0.52
2:L:120:PHE:HB2	2:L:135:VAL:HG22	1.90	0.52
1:H:134:PRO:HD2	1:H:218:THR:HG21	1.91	0.52
3:O:26:ARG:NH1	3:O:28:GLU:HB2	2.24	0.52
2:L:125:GLU:N	2:L:125:GLU:OE1	2.42	0.52
1:E:6:LEU:HD21	1:E:100:THR:HG23	1.92	0.52
1:E:15:LYS:HD3	1:E:128:SER:HA	1.91	0.51
1:H:26:ALA:HB3	1:H:79:ASP:HB3	1.93	0.51
1:C:53:ILE:HG13	1:C:60:VAL:HG22	1.93	0.51
2:D:191:HIS:HB2	2:D:194:TYR:HE1	1.74	0.51
2:D:117:VAL:HG21	2:D:198:VAL:HG11	1.92	0.51
1:C:166:THR:HG23	1:C:214:ASN:HB2	1.93	0.50
2:F:212:ASN:O	2:F:213:ARG:HG2	2.11	0.50
2:D:57:GLU:OE1	3:M:21:LYS:NZ	2.41	0.50
1:H:148:THR:HG22	1:H:198:PRO:HA	1.94	0.50
3:P:56:GLU:OE1	3:P:58:LYS:HD2	2.12	0.50
2:D:85:VAL:HG11	2:D:168:GLN:HB3	1.94	0.49
1:E:53:ILE:HG13	1:E:60:VAL:HG22	1.93	0.49
1:A:6:LEU:HA	1:A:26:ALA:HA	1.94	0.49
1:C:58:GLY:O	2:L:13:LEU:HA	2.12	0.49
2:D:120:PHE:HB2	2:D:135:VAL:HG22	1.94	0.49
2:F:189:GLU:HG3	2:F:213:ARG:HH22	1.77	0.49
3:N:26:ARG:HG2	3:N:28:GLU:H	1.78	0.49
1:C:108:THR:HG23	3:M:53:GLY:O	2.13	0.49
1:A:134:PRO:HD2	1:A:220:THR:HG21	1.94	0.48
1:A:210:ILE:HD11	1:A:223:ASP:OD2	2.13	0.48
1:A:210:ILE:HG13	1:A:224:LYS:C	2.34	0.48
1:E:104:LEU:HD12	3:O:58:LYS:HB2	1.95	0.48
1:E:134:PRO:HB3	1:E:160:TYR:HB3	1.95	0.48
2:B:115:PRO:HB3	2:B:141:PHE:HB3	1.94	0.48
2:F:109:LYS:HA	2:F:142:TYR:OH	2.14	0.48
2:L:121:PRO:HB3	2:L:211:PHE:CE2	2.49	0.48
2:D:115:PRO:HB3	2:D:141:PHE:HB3	1.95	0.48
2:D:189:GLU:HA	2:D:213:ARG:HH22	1.79	0.48
2:D:191:HIS:HB2	2:D:194:TYR:CE1	2.49	0.48
2:D:192:LYS:HG3	2:D:213:ARG:HB3	1.94	0.48
2:B:132:ALA:HB3	2:B:183:LEU:HD12	1.95	0.48
1:E:18:SER:O	1:E:88:LEU:HD23	2.14	0.48
3:P:51:LEU:HA	3:P:54:LEU:HD13	1.94	0.48
2:D:35:LEU:HD22	2:D:73:PHE:CG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:189:GLU:HA	2:F:213:ARG:HH22	1.79	0.47
1:H:197:VAL:HG21	1:H:207:TYR:OH	2.14	0.47
2:D:110:ARG:HH12	2:D:113:ALA:HB2	1.79	0.47
2:F:35:LEU:HD11	2:F:90:CYS:HB2	1.96	0.47
1:C:6:LEU:HD11	1:C:100:THR:HG23	1.97	0.47
3:P:30:VAL:O	3:P:34:ILE:HG13	2.14	0.47
1:H:152:GLY:HA2	1:H:167:TRP:CH2	2.50	0.47
2:B:110:ARG:HH21	2:B:113:ALA:HB2	1.80	0.46
3:P:48:ASP:OD2	3:P:52:LYS:NZ	2.48	0.46
2:F:148:VAL:HG22	2:F:198:VAL:HG22	1.97	0.46
3:P:31:GLU:HG2	3:P:51:LEU:HD11	1.97	0.46
2:D:157:GLN:HB3	2:D:160:ASN:HD21	1.80	0.46
3:N:31:GLU:HG2	3:N:51:LEU:HD21	1.96	0.46
2:F:193:VAL:HA	2:F:212:ASN:HA	1.98	0.45
2:F:115:PRO:HB3	2:F:141:PHE:HB3	1.97	0.45
1:H:35:ILE:HG23	1:H:54:ILE:HG12	1.97	0.45
3:O:26:ARG:O	3:O:29:GLU:CB	2.46	0.45
1:A:153:LEU:HD23	1:A:197:VAL:O	2.16	0.45
2:L:23:ILE:HD11	2:L:75:LEU:HD23	1.98	0.45
2:L:194:TYR:HB2	2:L:211:PHE:CE1	2.51	0.45
3:M:6:LYS:HB3	3:M:6:LYS:HE3	1.72	0.45
1:E:35:ILE:HG23	1:E:54:ILE:HG12	1.98	0.45
2:D:120:PHE:O	2:D:134:VAL:HG23	2.15	0.45
1:E:160:TYR:OH	1:E:193:LEU:HD23	2.17	0.45
2:B:37:TRP:HB2	2:B:50:ILE:HB	1.98	0.45
2:B:153:ASP:H	2:B:193:VAL:HB	1.82	0.44
2:F:91:GLN:HB2	2:F:100:PHE:CD2	2.52	0.44
1:C:207:GLN:HG3	1:C:209:TYR:CZ	2.52	0.44
3:M:15:LEU:HD12	3:M:16:LEU:HD12	1.99	0.44
2:D:156:LEU:HD12	2:D:156:LEU:N	2.33	0.44
1:H:12:GLU:OE1	1:H:14:LYS:NZ	2.46	0.44
2:D:124:ASP:OD1	2:D:124:ASP:N	2.48	0.44
2:L:39:GLN:HB2	2:L:49:LEU:HD11	1.98	0.44
3:M:30:VAL:O	3:M:34:ILE:HG13	2.18	0.44
3:O:27:PRO:C	3:O:29:GLU:N	2.70	0.44
2:D:165:VAL:HG22	2:D:177:LEU:CD2	2.48	0.44
1:H:20:VAL:HB	1:H:88:LEU:HD11	2.00	0.44
2:L:37:TRP:HB2	2:L:50:ILE:HB	2.00	0.44
1:H:164:THR:HG23	1:H:212:ASN:HB2	1.99	0.44
3:N:4:CYS:O	3:N:6:LYS:N	2.49	0.44
1:E:185:LEU:HB2	1:E:191:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASP:HA	1:A:190:LEU:HG	2.01	0.43
1:E:185:LEU:HD13	1:E:191:TYR:HE1	1.83	0.43
2:B:110:ARG:NH2	2:B:113:ALA:HB2	2.34	0.43
1:E:153:LEU:HD23	1:E:197:VAL:O	2.19	0.43
1:E:6:LEU:HD23	1:E:24:CYS:SG	2.59	0.43
2:F:35:LEU:HD22	2:F:73:PHE:CG	2.52	0.43
1:H:99:ALA:HB1	1:H:115:PHE:HB3	2.00	0.43
2:B:109:LYS:HA	2:B:142:TYR:OH	2.19	0.43
1:C:185:LEU:HD13	1:C:191:TYR:HE1	1.83	0.43
1:A:139:LEU:HB3	2:B:120:PHE:CD2	2.54	0.43
2:F:143:PRO:HG3	2:F:201:GLN:HE21	1.83	0.43
2:B:110:ARG:HD3	2:B:173:SER:HB2	2.01	0.42
2:L:109:LYS:HA	2:L:142:TYR:OH	2.19	0.42
3:N:30:VAL:O	3:N:34:ILE:HG13	2.19	0.42
2:B:51:TYR:O	2:B:55:ASN:HB2	2.18	0.42
1:E:20:VAL:O	1:E:84:HIS:HD2	2.01	0.42
2:B:160:ASN:ND2	2:B:181:LEU:HD21	2.35	0.42
1:H:6:LEU:HD21	1:H:100:THR:HG23	2.02	0.42
2:D:143:PRO:HG3	2:D:201:GLN:HE21	1.85	0.42
2:L:34:TYR:HB3	2:L:93:TYR:CE1	2.54	0.42
1:A:218:SER:OG	1:A:220:THR:OG1	2.34	0.42
1:C:99:ALA:HB1	1:C:115:PHE:HB3	2.01	0.42
1:E:209:TYR:O	1:E:226:VAL:N	2.52	0.42
2:L:110:ARG:NH2	2:L:113:ALA:HB2	2.35	0.42
2:L:115:PRO:HD3	2:L:200:HIS:ND1	2.35	0.42
3:O:26:ARG:NH1	3:O:28:GLU:H	2.18	0.42
1:A:110:TYR:CZ	1:A:113:HIS:HE1	2.38	0.42
2:L:122:PRO:HD3	2:L:134:VAL:HG22	2.01	0.42
2:D:34:TYR:HB3	2:D:93:TYR:CE2	2.55	0.42
1:A:204:LEU:HD22	1:A:204:LEU:H	1.85	0.41
1:H:6:LEU:HD23	1:H:24:CYS:SG	2.60	0.41
2:L:137:LEU:CD2	2:L:139:ASN:HB2	2.50	0.41
1:A:99:ALA:HB1	1:A:115:PHE:HB3	2.02	0.41
1:H:157:ASP:HA	1:H:188:LEU:HB3	2.01	0.41
3:P:2:SER:N	3:P:3:PRO:CD	2.84	0.41
3:P:11:ILE:HD13	3:P:11:ILE:HA	1.89	0.41
2:D:187:ASP:OD1	2:D:188:TYR:N	2.53	0.41
2:L:183:LEU:HD23	2:L:183:LEU:HA	1.93	0.41
2:D:68:GLY:HA3	2:D:73:PHE:HA	2.03	0.41
2:L:156:LEU:H	2:L:156:LEU:HD12	1.86	0.41
1:A:25:GLN:O	1:A:79:ASP:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:137:LEU:HD21	2:L:139:ASN:HB2	2.02	0.41
1:C:181:PHE:CZ	2:D:178:SER:HB3	2.55	0.41
2:D:138:LEU:HD13	2:D:177:LEU:HB3	2.01	0.41
2:D:152:VAL:HG21	2:D:157:GLN:NE2	2.36	0.41
1:A:132:LYS:HD3	1:A:133:GLY:O	2.20	0.41
1:H:116:ASP:OD2	3:P:21:LYS:NZ	2.54	0.40
2:L:142:TYR:CD1	2:L:143:PRO:HA	2.56	0.40
2:D:160:ASN:OD1	2:D:160:ASN:N	2.53	0.40
1:E:137:PHE:HA	1:E:138:PRO:HD3	1.92	0.40
1:H:152:GLY:HA2	1:H:167:TRP:HH2	1.86	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	208/241 (86%)	199 (96%)	8 (4%)	1 (0%)	29 68
1	C	211/241 (88%)	200 (95%)	11 (5%)	0	100 100
1	E	209/241 (87%)	201 (96%)	8 (4%)	0	100 100
1	H	208/241 (86%)	201 (97%)	6 (3%)	1 (0%)	29 68
2	B	206/225 (92%)	197 (96%)	8 (4%)	1 (0%)	29 68
2	D	198/225 (88%)	192 (97%)	5 (2%)	1 (0%)	29 68
2	F	198/225 (88%)	192 (97%)	5 (2%)	1 (0%)	29 68
2	L	209/225 (93%)	203 (97%)	5 (2%)	1 (0%)	29 68
3	M	57/71 (80%)	54 (95%)	2 (4%)	1 (2%)	8 37
3	N	56/71 (79%)	51 (91%)	5 (9%)	0	100 100
3	O	57/71 (80%)	53 (93%)	3 (5%)	1 (2%)	8 37
3	P	56/71 (79%)	51 (91%)	5 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1873/2148 (87%)	1794 (96%)	71 (4%)	8 (0%)	34 72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	32	VAL
3	O	23	GLY
2	D	32	VAL
2	B	32	VAL
2	L	32	VAL
1	A	28	GLY
1	H	28	GLY
3	M	3	PRO

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	173/205 (84%)	169 (98%)	4 (2%)	50 80
1	C	178/205 (87%)	172 (97%)	6 (3%)	37 72
1	E	174/205 (85%)	170 (98%)	4 (2%)	50 80
1	H	177/205 (86%)	172 (97%)	5 (3%)	43 77
2	B	177/198 (89%)	172 (97%)	5 (3%)	43 77
2	D	177/198 (89%)	176 (99%)	1 (1%)	86 95
2	F	172/198 (87%)	168 (98%)	4 (2%)	50 80
2	L	177/198 (89%)	174 (98%)	3 (2%)	60 85
3	M	47/63 (75%)	46 (98%)	1 (2%)	53 82
3	N	52/63 (82%)	51 (98%)	1 (2%)	57 84
3	O	50/63 (79%)	45 (90%)	5 (10%)	7 29
3	P	51/63 (81%)	48 (94%)	3 (6%)	19 54
All	All	1605/1864 (86%)	1563 (97%)	42 (3%)	46 78

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	TYR
1	A	190	LEU
1	A	212	ASN
1	A	224	LYS
2	B	35	LEU
2	B	83	GLU
2	B	128	LYS
2	B	183	LEU
2	B	188	TYR
1	C	15	LYS
1	C	110	TYR
1	C	117	ASN
1	C	139	LEU
1	C	159	ASP
1	C	223	ASP
2	D	156	LEU
1	E	21	MET
1	E	89	ARG
1	E	110	TYR
1	E	159	ASP
2	F	13	LEU
2	F	56	LEU
2	F	156	LEU
2	F	160	ASN
1	H	107	SER
1	H	110	TYR
1	H	209	CYS
1	H	210	ASN
1	H	221	ASP
2	L	56	LEU
2	L	83	GLU
2	L	183	LEU
3	M	46	CYS
3	N	46	CYS
3	O	26	ARG
3	O	29	GLU
3	O	32	GLU
3	O	33	ARG
3	O	38	LEU
3	P	24	CYS
3	P	26	ARG
3	P	46	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	139	ASN

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 monosaccharides 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	212/241 (87%)	0.21	12 (5%) 23 8	46, 89, 135, 169	0
1	C	215/241 (89%)	0.21	4 (1%) 66 37	51, 100, 165, 200	0
1	E	215/241 (89%)	0.15	7 (3%) 46 20	46, 101, 160, 194	0
1	H	212/241 (87%)	0.22	9 (4%) 36 14	50, 103, 190, 249	0
2	B	210/225 (93%)	0.01	6 (2%) 51 23	52, 84, 159, 176	0
2	D	206/225 (91%)	0.00	7 (3%) 45 19	36, 80, 149, 166	0
2	F	206/225 (91%)	-0.02	3 (1%) 73 46	50, 85, 189, 230	0
2	L	211/225 (93%)	0.03	7 (3%) 46 20	46, 86, 172, 190	0
3	M	59/71 (83%)	0.02	1 (1%) 70 41	89, 130, 160, 163	0
3	N	58/71 (81%)	-0.05	1 (1%) 70 41	76, 113, 148, 156	0
3	O	59/71 (83%)	-0.03	1 (1%) 70 41	82, 131, 152, 168	0
3	P	58/71 (81%)	-0.13	0 100 100	74, 114, 141, 146	0
All	All	1921/2148 (89%)	0.08	58 (3%) 50 22	36, 95, 165, 249	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	138	PRO	6.2
1	A	138	PRO	5.5
2	D	123	SER	5.5
1	C	135	SER	4.9
2	L	123	SER	4.3
2	L	150	TRP	4.2
1	H	137	PHE	4.2
1	A	137	PHE	4.1
2	B	125	GLU	3.9
1	E	217	PRO	3.8
2	D	124	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	211	PHE	3.3
2	B	124	ASP	3.2
1	H	215	PRO	3.1
2	B	150	TRP	3.0
1	A	135	SER	3.0
2	D	122	PRO	3.0
2	D	181	LEU	3.0
1	H	154	LEU	3.0
2	D	195	ALA	3.0
2	D	128	LYS	2.9
1	H	136	VAL	2.8
1	H	135	SER	2.8
3	O	42	GLY	2.8
1	H	151	LEU	2.7
2	D	212	ASN	2.7
1	A	153	LEU	2.7
2	L	181	LEU	2.6
1	A	219	ASN	2.6
2	B	135	VAL	2.6
2	F	124	ASP	2.6
1	A	169	TRP	2.5
1	A	159	ASP	2.5
1	H	159	PHE	2.4
1	E	160	TYR	2.4
1	E	226	VAL	2.4
1	A	217	PRO	2.4
1	C	165	VAL	2.3
2	L	135	VAL	2.3
2	L	125	GLU	2.3
1	A	155	CYS	2.3
1	A	136	VAL	2.3
1	E	173	ALA	2.2
2	L	121	PRO	2.2
3	N	41	MET	2.2
1	A	139	LEU	2.1
2	B	134	VAL	2.1
1	C	154	GLY	2.1
1	E	138	PRO	2.1
1	E	152	ALA	2.1
1	E	213	VAL	2.0
1	C	228	PRO	2.0
3	M	42	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	L	133	SER	2.0
2	F	128	LYS	2.0
1	A	156	LEU	2.0
2	B	183	LEU	2.0
1	H	193	SER	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 monosaccharides 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.