Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 04:08 am BST

PDB ID	:	3UTZ
Title	:	Endogenous-like inhibitory antibodies targeting activated metalloproteinase motifs show therapeutic potential
Authors	:	Sela-Passwell, N.; Kikkeri, R.; Dym, O.; Rozenberg, H.; Margalit, R.; Arad-Yellin, R.; Eisenstein, M.; Brenner, O.; Shoham, T.; Danon, T.; Shanzer, A.; Sagi, I.; Israel Structural Proteomics Center (ISPC)
Deposited on	:	2011-11-27
Resolution	:	2.18 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 (i) symbol.

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

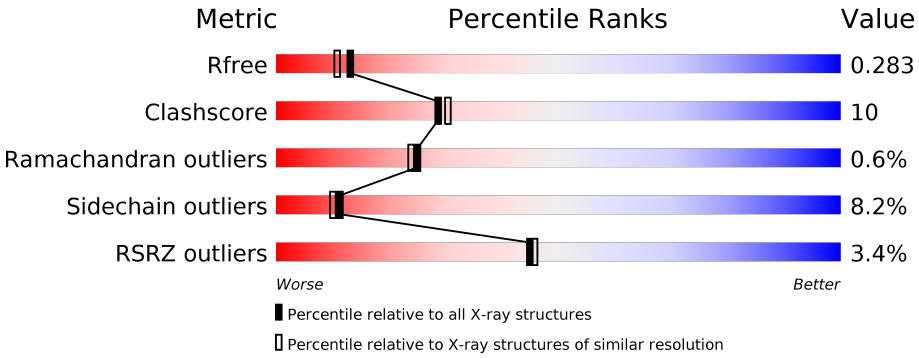
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 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	219	2% 74% 22%
1	D	219	3% 79% 17%
1	E	219	8% 78% 15%
2	B	225	2% 76% 17%
2	C	225	% 72% 19% 5%
2	F	225	4% 72% 20% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9465 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.

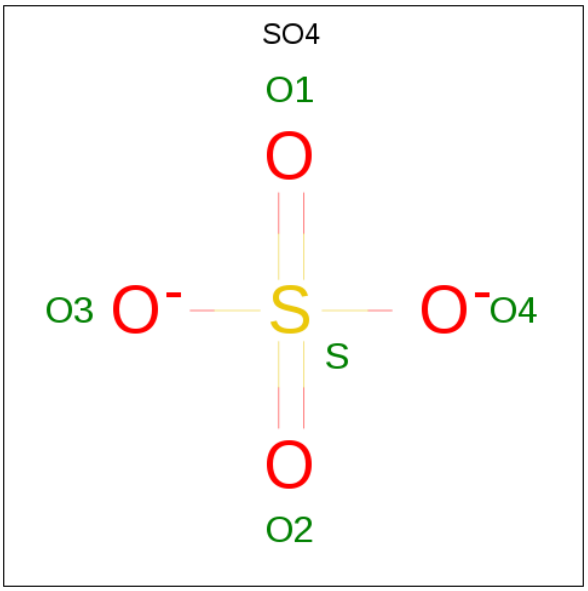
- Molecule 1 is a protein called Metalloproteinase, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1604	1009	267	323	5			
1	D	212	Total	C	N	O	S	0	0	0
			1545	976	254	310	5			
1	E	212	Total	C	N	O	S	0	0	0
			1542	976	255	306	5			

- Molecule 2 is a protein called Metalloproteinase, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1605	1021	263	315	6			
2	C	214	Total	C	N	O	S	0	0	0
			1556	989	256	305	6			
2	F	213	Total	C	N	O	S	0	0	0
			1558	990	253	309	6			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total O 2 2	0	0
4	C	1	Total O 1 1	0	0

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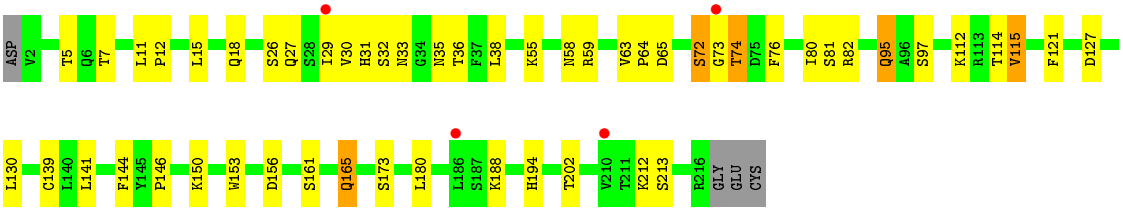
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

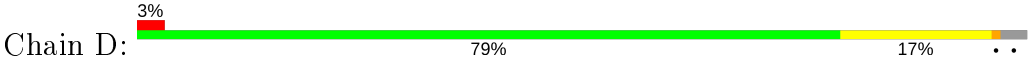
- Molecule 1: Metalloproteinase, light chain

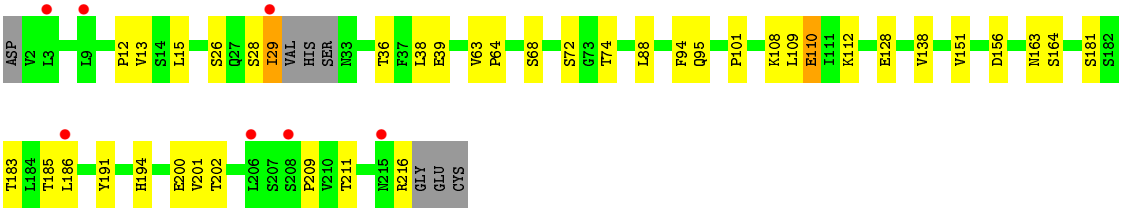
Chain A:



- Molecule 1: Metalloproteinase, light chain

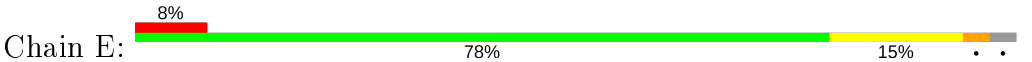
Chain D:

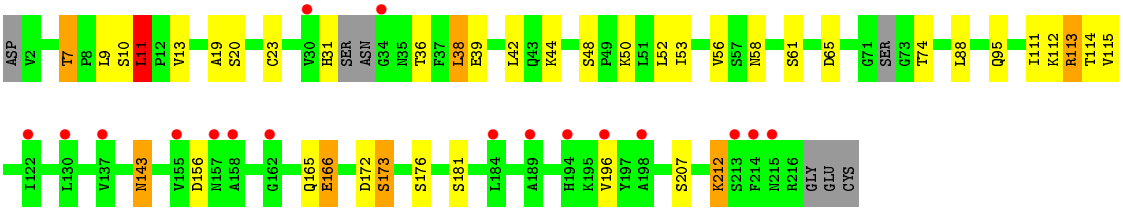




- Molecule 1: Metalloproteinase, light chain

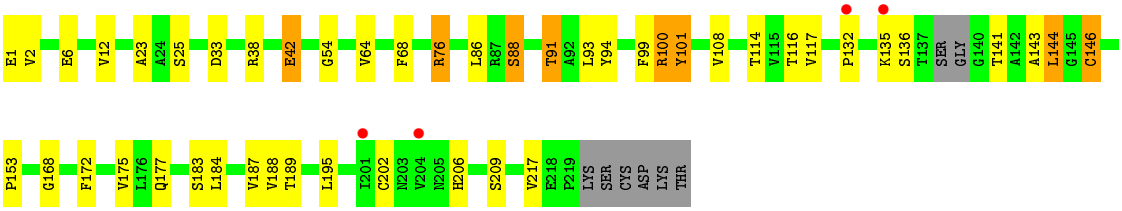
Chain E:



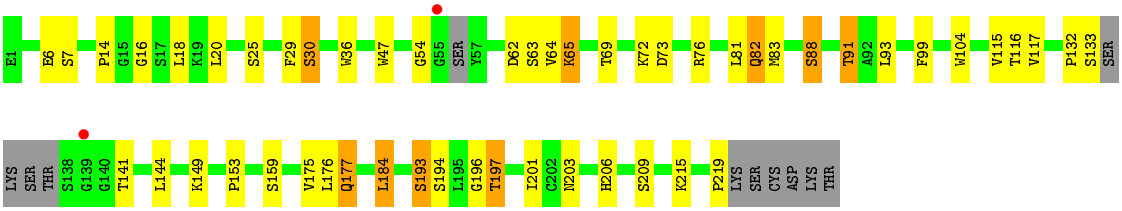


- Molecule 2: Metalloproteinase, heavy chain

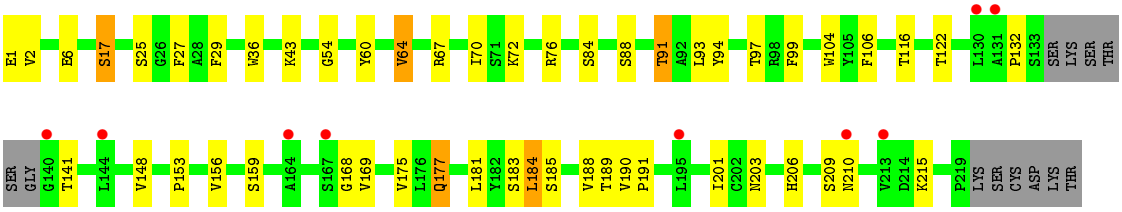
Chain B:



• Molecule 2: Metalloproteinase, heavy chain



• Molecule 2: Metalloproteinase, heavy chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.09Å 108.37Å 86.47Å 90.00° 111.91° 90.00°	Depositor
Resolution (Å)	41.27 – 2.18 41.27 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.5 (41.27-2.18) 98.4 (41.27-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.228 , 0.288 0.228 , 0.283	Depositor DCC
R_{free} test set	3655 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9465	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.89	1/1641 (0.1%)	0.87	1/2238 (0.0%)
1	D	1.08	2/1580 (0.1%)	0.92	0/2159
1	E	0.92	0/1576	0.84	1/2151 (0.0%)
2	B	1.01	1/1646 (0.1%)	0.96	4/2248 (0.2%)
2	C	1.00	0/1596	0.89	0/2183
2	F	1.05	0/1599	0.89	1/2187 (0.0%)
All	All	0.99	4/9638 (0.0%)	0.90	7/13166 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	23	ALA	CA-CB	5.64	1.64	1.52
1	D	138	VAL	CB-CG1	5.20	1.63	1.52
1	D	95	GLN	CB-CG	-5.11	1.38	1.52
1	A	144	PHE	CE2-CZ	5.06	1.47	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	146	CYS	CA-CB-SG	6.58	125.84	114.00
1	E	11	LEU	CA-CB-CG	5.85	128.75	115.30
2	B	76	ARG	NE-CZ-NH2	-5.83	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	32	SER	N-CA-C	-5.77	95.41	111.00
2	B	76	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	B	38	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	F	76	ARG	NE-CZ-NH2	-5.17	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	7	SER	Peptide

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	1604	0	1503	32	0
1	D	1545	0	1418	25	0
1	E	1542	0	1426	30	0
2	B	1605	0	1535	30	0
2	C	1556	0	1452	31	0
2	F	1558	0	1453	39	0
3	B	25	0	0	1	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	F	10	0	0	2	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	9465	0	8787	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (177) 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)
2:B:146:CYS:SG	2:B:202:CYS:SG	1.16	1.15
1:E:113:ARG:HH11	1:E:113:ARG:CG	1.58	1.08
2:B:146:CYS:SG	2:B:202:CYS:CB	2.43	1.07
2:F:184:LEU:HD12	2:F:184:LEU:C	1.81	1.01
1:E:113:ARG:HH11	1:E:113:ARG:HG3	0.83	0.99
1:E:113:ARG:HG3	1:E:113:ARG:NH1	1.61	0.98
2:C:88:SER:O	2:C:91:THR:HG23	1.63	0.97
1:D:29:ILE:HG23	1:D:29:ILE:O	1.74	0.87
1:D:163:ASN:ND2	1:D:186:LEU:HD21	1.90	0.86
1:A:15:LEU:HD12	1:A:15:LEU:H	1.42	0.84
2:F:184:LEU:HD12	2:F:184:LEU:O	1.80	0.81
1:D:29:ILE:CG2	1:D:29:ILE:O	2.30	0.79
2:F:184:LEU:CD1	2:F:184:LEU:C	2.51	0.78
1:E:143:ASN:N	1:E:143:ASN:HD22	1.84	0.76
2:C:132:PRO:HG2	2:C:219:PRO:HB3	1.68	0.74
1:D:15:LEU:HD12	1:D:15:LEU:H	1.49	0.74
1:D:163:ASN:HD22	1:D:186:LEU:HD21	1.51	0.73
2:B:54:GLY:HA3	3:B:227:SO4:O1	1.88	0.73
1:A:30:VAL:HG22	1:A:36:THR:HG22	1.69	0.73
1:A:59:ARG:NH1	1:A:65:ASP:HA	2.04	0.73
1:D:185:THR:O	1:D:186:LEU:HD23	1.91	0.71
1:A:29:ILE:HD11	1:A:76:PHE:CZ	2.26	0.71
2:C:153:PRO:O	2:C:206:HIS:HE1	1.73	0.70
1:A:30:VAL:HG22	1:A:36:THR:CG2	2.21	0.70
2:F:190:VAL:HB	2:F:191:PRO:HD2	1.75	0.67
2:B:153:PRO:O	2:B:206:HIS:HE1	1.77	0.67
1:D:13:VAL:HG11	1:D:109:LEU:HD11	1.77	0.67
1:E:143:ASN:H	1:E:143:ASN:HD22	1.40	0.67
1:E:172:ASP:OD1	1:E:173:SER:N	2.28	0.67
2:C:91:THR:HG22	2:C:117:VAL:H	1.59	0.67
1:E:113:ARG:NH1	1:E:114:THR:O	2.29	0.65
2:F:201:ILE:HA	2:F:215:LYS:O	1.96	0.65
2:B:42:GLU:N	2:B:42:GLU:OE2	2.29	0.65
1:D:15:LEU:N	1:D:15:LEU:HD12	2.12	0.65
1:D:163:ASN:HD22	1:D:186:LEU:CD2	2.09	0.65
2:F:153:PRO:O	2:F:206:HIS:HE1	1.80	0.64
1:A:72:SER:O	1:A:74:THR:N	2.30	0.64
1:A:59:ARG:HH11	1:A:65:ASP:HA	1.61	0.64
2:F:88:SER:O	2:F:91:THR:HG23	1.97	0.64
2:B:88:SER:O	2:B:91:THR:HG23	1.98	0.63
1:A:213:SER:O	2:B:135:LYS:HD2	1.98	0.62
1:A:31:HIS:O	1:A:33:ASN:N	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:HB3	1:A:202:THR:HB	1.81	0.61
2:C:29:PHE:CE2	2:C:72:LYS:HE2	2.35	0.61
2:F:2:VAL:HG13	2:F:27:PHE:CD1	2.36	0.61
1:E:113:ARG:CG	1:E:113:ARG:NH1	2.33	0.60
1:D:156:ASP:OD2	1:D:194:HIS:HB3	2.01	0.60
1:E:44:LYS:HE3	1:E:50:LYS:HE2	1.83	0.60
2:B:2:VAL:CG1	2:B:108:VAL:HG21	2.32	0.60
1:D:15:LEU:CD1	1:D:15:LEU:H	2.15	0.59
1:D:151:VAL:HG22	1:D:201:VAL:HG22	1.85	0.58
2:F:6:GLU:OE2	2:F:94:TYR:O	2.21	0.58
2:B:100:ARG:NH2	2:B:101:TYR:CE2	2.72	0.58
1:A:30:VAL:HA	1:A:36:THR:HG22	1.85	0.58
1:D:38:LEU:HG	1:D:39:GLU:N	2.18	0.58
2:B:2:VAL:HG11	2:B:108:VAL:HG21	1.85	0.57
2:C:93:LEU:HD23	2:C:93:LEU:C	2.27	0.55
1:E:143:ASN:ND2	1:E:143:ASN:N	2.54	0.55
1:E:11:LEU:HD12	1:E:13:VAL:CG2	2.36	0.55
2:C:83:MET:CE	2:C:115:VAL:HG21	2.37	0.55
2:F:54:GLY:HA3	3:F:227:SO4:O3	2.06	0.55
2:B:91:THR:HB	2:B:116:THR:HA	1.88	0.54
1:E:13:VAL:HG21	1:E:19:ALA:HB2	1.90	0.54
2:C:99:PHE:CZ	2:C:104:TRP:HA	2.43	0.53
1:E:38:LEU:HG	1:E:39:GLU:N	2.23	0.53
1:E:113:ARG:NH1	1:E:114:THR:N	2.57	0.53
2:F:169:VAL:HG22	2:F:188:VAL:HB	1.91	0.53
2:C:18:LEU:O	2:C:83:MET:N	2.32	0.53
1:E:53:ILE:HA	1:E:58:ASN:O	2.09	0.52
2:F:122:THR:HG22	2:F:209:SER:HB3	1.91	0.52
1:E:113:ARG:HH11	1:E:113:ARG:CB	2.20	0.52
1:D:128:GLU:OE2	2:C:215:LYS:HE3	2.09	0.52
2:C:175:VAL:HG12	2:C:176:LEU:N	2.24	0.52
2:B:206:HIS:HD2	2:B:209:SER:OG	1.93	0.52
1:E:166:GLU:HA	1:E:181:SER:O	2.09	0.52
2:C:30:SER:OG	1:E:61:SER:HB3	2.10	0.52
2:F:29:PHE:CE2	2:F:72:LYS:HE2	2.46	0.51
2:F:168:GLY:O	2:F:188:VAL:HG23	2.10	0.51
1:A:15:LEU:CD1	1:A:15:LEU:H	2.17	0.50
2:F:177:GLN:HG2	2:F:181:LEU:O	2.11	0.50
2:B:12:VAL:HG11	2:B:86:LEU:HD13	1.94	0.50
2:C:196:GLY:O	2:C:197:THR:O	2.30	0.50
1:A:81:SER:O	1:A:82:ARG:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:THR:CG2	2:C:117:VAL:H	2.23	0.49
2:F:159:SER:OG	2:F:203:ASN:HB2	2.12	0.49
2:C:193:SER:OG	2:C:193:SER:O	2.30	0.49
1:A:55:LYS:HB2	1:A:58:ASN:HD22	1.78	0.49
1:A:95:GLN:OE1	1:A:97:SER:N	2.45	0.49
1:E:165:GLN:NE2	2:F:175:VAL:CG1	2.76	0.49
2:B:168:GLY:O	2:B:188:VAL:HA	2.13	0.49
2:B:177:GLN:HE21	2:B:183:SER:HB2	1.79	0.48
2:B:172:PHE:HE1	2:B:187:VAL:HG22	1.78	0.48
1:D:94:PHE:CZ	1:D:101:PRO:HB2	2.48	0.48
2:F:184:LEU:HD12	2:F:185:SER:N	2.26	0.48
2:B:64:VAL:HG13	2:B:68:PHE:HB2	1.95	0.48
1:D:29:ILE:HD12	1:D:29:ILE:HA	1.58	0.48
2:B:143:ALA:HB2	2:B:189:THR:HG22	1.95	0.48
2:F:188:VAL:HG22	2:F:189:THR:N	2.29	0.48
1:A:165:GLN:HE21	1:A:165:GLN:HB3	1.47	0.48
2:C:83:MET:HE1	2:C:115:VAL:HG21	1.94	0.48
2:C:69:THR:HB	2:C:82:GLN:HB2	1.96	0.47
2:F:29:PHE:CZ	2:F:72:LYS:HE2	2.49	0.47
1:D:12:PRO:HB2	1:D:112:LYS:HD2	1.96	0.47
1:E:11:LEU:HD12	1:E:13:VAL:HG23	1.96	0.47
1:D:88:LEU:HA	1:D:109:LEU:HD23	1.96	0.47
1:E:7:THR:HG22	1:E:7:THR:O	2.15	0.47
1:E:88:LEU:HD21	1:E:111:ILE:HD11	1.96	0.47
1:A:31:HIS:C	1:A:33:ASN:H	2.15	0.46
1:E:11:LEU:CD1	1:E:13:VAL:CG2	2.94	0.46
2:F:148:VAL:HG11	2:F:156:VAL:HG11	1.97	0.46
1:A:33:ASN:HD21	1:A:35:ASN:HD22	1.62	0.46
1:A:127:ASP:HA	1:A:130:LEU:HD12	1.98	0.46
1:A:31:HIS:CD2	1:A:97:SER:O	2.69	0.46
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.51	0.46
1:D:164:SER:HA	1:D:183:THR:O	2.16	0.46
1:E:165:GLN:HE21	2:F:175:VAL:HG11	1.81	0.46
2:C:14:PRO:C	2:C:16:GLY:H	2.19	0.46
2:B:25:SER:HB3	2:F:25:SER:HB3	1.97	0.45
2:F:17:SER:HB2	2:F:84:SER:HA	1.98	0.45
2:F:99:PHE:CZ	2:F:104:TRP:HA	2.51	0.45
1:D:108:LYS:HG2	1:D:110:GLU:OE1	2.17	0.45
2:C:184:LEU:HD12	2:C:184:LEU:C	2.37	0.44
1:E:113:ARG:HD2	1:E:176:SER:HB2	1.99	0.44
2:C:91:THR:HB	2:C:116:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:206:HIS:HD2	2:F:209:SER:OG	2.00	0.44
2:F:43:LYS:HA	2:F:43:LYS:HD3	1.84	0.44
2:C:83:MET:HE1	2:C:115:VAL:HG11	2.00	0.44
2:F:177:GLN:NE2	2:F:183:SER:HB2	2.32	0.44
2:F:67:ARG:HB3	2:F:84:SER:O	2.18	0.44
2:F:209:SER:O	2:F:210:ASN:C	2.54	0.44
2:B:6:GLU:OE2	2:B:94:TYR:O	2.35	0.44
1:D:63:VAL:HA	1:D:64:PRO:HD3	1.73	0.44
1:E:165:GLN:NE2	2:F:175:VAL:HG11	2.32	0.43
2:C:62:ASP:HA	2:C:65:LYS:HD3	2.01	0.43
2:C:177:GLN:HE21	2:C:177:GLN:HB2	1.53	0.43
1:A:115:VAL:HG12	1:A:146:PRO:HD3	2.00	0.43
2:B:132:PRO:HD3	2:B:144:LEU:HB3	2.00	0.43
2:B:91:THR:HG22	2:B:117:VAL:H	1.83	0.42
2:C:64:VAL:O	2:C:65:LYS:C	2.57	0.42
1:A:18:GLN:HA	1:A:80:ILE:O	2.20	0.42
2:B:168:GLY:O	2:B:188:VAL:HG23	2.19	0.42
1:A:165:GLN:HG3	2:B:175:VAL:HG21	2.01	0.42
1:A:156:ASP:OD2	1:A:194:HIS:HB3	2.20	0.42
2:B:76:ARG:NH1	3:F:226:SO4:O1	2.52	0.42
2:F:60:TYR:HB3	2:F:64:VAL:HG12	2.00	0.42
1:A:55:LYS:CB	1:A:58:ASN:HD22	2.33	0.42
2:B:195:LEU:HA	2:B:195:LEU:HD23	1.83	0.42
2:B:42:GLU:CD	2:B:42:GLU:H	2.22	0.42
2:C:159:SER:OG	2:C:203:ASN:HB2	2.20	0.41
2:C:20:LEU:HB2	2:C:81:LEU:HB3	2.02	0.41
1:A:59:ARG:NH1	1:A:65:ASP:CA	2.77	0.41
1:A:63:VAL:HA	1:A:64:PRO:HD2	1.95	0.41
1:E:156:ASP:HA	1:E:196:VAL:HB	2.02	0.41
2:F:97:THR:OG1	2:F:106:PHE:HB3	2.19	0.41
2:F:36:TRP:HD1	2:F:70:ILE:HD12	1.85	0.41
1:D:13:VAL:CG1	1:D:109:LEU:HD11	2.49	0.41
2:C:73:ASP:CB	2:C:76:ARG:HG3	2.51	0.41
1:A:12:PRO:HB2	1:A:112:LYS:HE3	2.03	0.41
1:E:143:ASN:H	1:E:143:ASN:ND2	2.11	0.41
2:C:206:HIS:HD2	2:C:209:SER:OG	2.04	0.41
2:F:122:THR:CG2	2:F:209:SER:HB3	2.50	0.41
1:A:139:CYS:HB2	1:A:153:TRP:CH2	2.56	0.41
2:C:29:PHE:CE2	2:C:72:LYS:HG2	2.56	0.41
1:D:191:TYR:CZ	1:D:216:ARG:HG3	2.56	0.41
1:E:212:LYS:HA	1:E:212:LYS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD22	1:A:180:LEU:HD22	2.03	0.41
2:B:12:VAL:O	2:B:117:VAL:HA	2.21	0.41
1:A:121:PHE:HB3	2:B:136:SER:HA	2.02	0.40
1:D:101:PRO:HD2	2:C:47:TRP:CE3	2.57	0.40
2:F:184:LEU:CD1	2:F:185:SER:N	2.83	0.40
2:B:100:ARG:NH2	2:B:101:TYR:CD2	2.89	0.40
1:D:200:GLU:HG3	1:D:211:THR:OG1	2.21	0.40
1:E:42:LEU:HB2	1:E:52:LEU:HD11	2.04	0.40
2:F:168:GLY:C	2:F:188:VAL:HG23	2.42	0.40
1:A:114:THR:O	1:A:115:VAL:C	2.58	0.40
2:F:177:GLN:HG2	2:F:177:GLN:H	1.51	0.40
2:F:91:THR:HB	2:F:116:THR:HA	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	213/219 (97%)	203 (95%)	8 (4%)	2 (1%)	17 15
1	D	208/219 (95%)	200 (96%)	7 (3%)	1 (0%)	29 28
1	E	206/219 (94%)	195 (95%)	10 (5%)	1 (0%)	29 28
2	B	213/225 (95%)	207 (97%)	6 (3%)	0	100 100
2	C	208/225 (92%)	193 (93%)	12 (6%)	3 (1%)	11 8
2	F	209/225 (93%)	197 (94%)	11 (5%)	1 (0%)	29 28
All	All	1257/1332 (94%)	1195 (95%)	54 (4%)	8 (1%)	25 24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLY

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Mol	Chain	Res	Type
2	C	197	THR
2	C	54	GLY
2	C	88	SER
2	F	132	PRO
1	D	209	PRO
1	E	56	VAL
1	A	115	VAL

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	177/195 (91%)	163 (92%)	14 (8%)	12 11
1	D	164/195 (84%)	154 (94%)	10 (6%)	18 19
1	E	164/195 (84%)	143 (87%)	21 (13%)	4 3
2	B	174/192 (91%)	160 (92%)	14 (8%)	12 11
2	C	164/192 (85%)	148 (90%)	16 (10%)	8 6
2	F	165/192 (86%)	157 (95%)	8 (5%)	25 29
All	All	1008/1161 (87%)	925 (92%)	83 (8%)	11 10

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	7	THR
1	A	11	LEU
1	A	26	SER
1	A	27	GLN
1	A	38	LEU
1	A	72	SER
1	A	74	THR
1	A	95	GLN
1	A	161	SER
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	173	SER
1	A	188	LYS
1	A	212	LYS
2	B	1	GLU
2	B	33	ASP
2	B	42	GLU
2	B	88	SER
2	B	91	THR
2	B	93	LEU
2	B	99	PHE
2	B	100	ARG
2	B	101	TYR
2	B	114	THR
2	B	141	THR
2	B	144	LEU
2	B	184	LEU
2	B	217	VAL
1	D	26	SER
1	D	28	SER
1	D	29	ILE
1	D	36	THR
1	D	68	SER
1	D	72	SER
1	D	74	THR
1	D	110	GLU
1	D	181	SER
1	D	202	THR
2	C	6	GLU
2	C	25	SER
2	C	30	SER
2	C	63	SER
2	C	65	LYS
2	C	82	GLN
2	C	91	THR
2	C	133	SER
2	C	141	THR
2	C	144	LEU
2	C	149	LYS
2	C	177	GLN
2	C	184	LEU
2	C	193	SER
2	C	194	SER

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Mol	Chain	Res	Type
2	C	201	ILE
1	E	7	THR
1	E	9	LEU
1	E	10	SER
1	E	11	LEU
1	E	20	SER
1	E	23	CYS
1	E	31	HIS
1	E	36	THR
1	E	38	LEU
1	E	48	SER
1	E	65	ASP
1	E	74	THR
1	E	95	GLN
1	E	112	LYS
1	E	113	ARG
1	E	115	VAL
1	E	143	ASN
1	E	166	GLU
1	E	173	SER
1	E	207	SER
1	E	212	LYS
2	F	1	GLU
2	F	17	SER
2	F	64	VAL
2	F	91	THR
2	F	93	LEU
2	F	141	THR
2	F	177	GLN
2	F	184	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	35	ASN
1	A	58	ASN
1	A	143	ASN
1	A	165	GLN
1	A	194	HIS
2	B	77	ASN
2	B	82	GLN

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Mol	Chain	Res	Type
2	B	177	GLN
2	B	206	HIS
1	D	43	GLN
1	D	142	ASN
1	D	194	HIS
2	C	39	GLN
2	C	170	HIS
2	C	177	GLN
2	C	205	ASN
2	C	206	HIS
1	E	43	GLN
1	E	143	ASN
1	E	157	ASN
1	E	165	GLN
1	E	194	HIS
2	F	39	GLN
2	F	77	ASN
2	F	206	HIS

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

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	B	226	-	4,4,4	0.20	0	6,6,6	0.38	0
3	SO4	B	229	-	4,4,4	0.17	0	6,6,6	0.24	0
3	SO4	F	226	-	4,4,4	0.57	0	6,6,6	0.74	0
3	SO4	D	221	-	4,4,4	0.33	0	6,6,6	0.43	0
3	SO4	B	228	-	4,4,4	0.10	0	6,6,6	0.27	0
3	SO4	D	220	-	4,4,4	0.23	0	6,6,6	0.43	0
3	SO4	B	227	-	4,4,4	0.23	0	6,6,6	0.59	0
3	SO4	B	230	-	4,4,4	0.31	0	6,6,6	0.30	0
3	SO4	F	227	-	4,4,4	0.22	0	6,6,6	0.36	0
3	SO4	C	226	-	4,4,4	0.38	0	6,6,6	1.92	2 (33%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	226	SO4	O3-S-O1	-3.23	92.43	109.31
3	C	226	SO4	O3-S-O2	2.04	119.96	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	226	SO4	1	0
3	B	227	SO4	1	0
3	F	227	SO4	1	0

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, 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	215/219 (98%)	0.39	4 (1%)	66	67	39, 57, 72, 86	0
1	D	212/219 (96%)	0.31	7 (3%)	46	47	34, 51, 71, 82	0
1	E	212/219 (96%)	0.59	17 (8%)	12	12	36, 58, 80, 84	0
2	B	217/225 (96%)	0.30	4 (1%)	68	69	36, 50, 68, 81	0
2	C	214/225 (95%)	0.30	2 (0%)	84	84	36, 55, 70, 80	0
2	F	213/225 (94%)	0.56	9 (4%)	36	37	33, 51, 79, 85	0
All	All	1283/1332 (96%)	0.41	43 (3%)	45	46	33, 54, 75, 86	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	139	GLY	4.7
1	E	196	VAL	4.6
2	F	195	LEU	4.5
2	F	213	VAL	4.5
1	D	29	ILE	4.4
1	E	189	ALA	4.1
1	E	30	VAL	4.0
1	A	73	GLY	3.8
2	F	144	LEU	3.8
1	E	137	VAL	3.7
1	E	214	PHE	3.7
1	E	184	LEU	3.6
2	F	164	ALA	3.4
2	F	131	ALA	3.3
2	B	201	ILE	3.0
1	D	208	SER	2.9
1	E	155	VAL	2.8
1	E	215	ASN	2.8
2	F	140	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	167	SER	2.8
1	D	215	ASN	2.7
1	E	122	ILE	2.7
1	A	186	LEU	2.7
1	E	213	SER	2.6
1	E	194	HIS	2.6
1	E	162	GLY	2.5
2	F	210	ASN	2.4
1	E	198	ALA	2.4
1	E	157	ASN	2.4
2	C	55	GLY	2.3
1	E	130	LEU	2.3
1	E	158	ALA	2.3
1	D	186	LEU	2.3
2	B	204	VAL	2.3
1	D	3	LEU	2.2
1	A	210	VAL	2.2
1	E	34	GLY	2.1
2	B	132	PRO	2.1
1	D	9	LEU	2.1
2	F	130	LEU	2.0
2	B	135	LYS	2.0
1	A	29	ILE	2.0
1	D	206	LEU	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	229	5/5	0.87	0.12	94,95,96,97	0
3	SO4	B	230	5/5	0.88	0.11	90,90,93,93	0
3	SO4	B	228	5/5	0.91	0.10	95,97,98,98	0
3	SO4	D	220	5/5	0.92	0.18	83,83,86,86	0
3	SO4	F	227	5/5	0.92	0.12	88,88,89,91	0
3	SO4	D	221	5/5	0.94	0.12	86,86,89,90	0
3	SO4	B	227	5/5	0.94	0.11	81,84,85,86	0
3	SO4	C	226	5/5	0.97	0.22	53,54,59,59	0
3	SO4	F	226	5/5	0.99	0.15	37,38,39,42	0
3	SO4	B	226	5/5	0.99	0.08	56,56,58,59	0

6.5 Other polymers (i)

There are no such residues in this entry.