Full wwPDB X-ray Structure Validation Report (i)

Sep 29, 2024 – 12:04 AM EDT

PDB ID	:	1SU3
Title	:	X-ray structure of human proMMP-1: New insights into collagenase action
Authors	:	Jozic, D.; Bourenkov, G.; Lim, N.H.; Nagase, H.; Bode, W.; Maskos, K.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2004-03-26
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

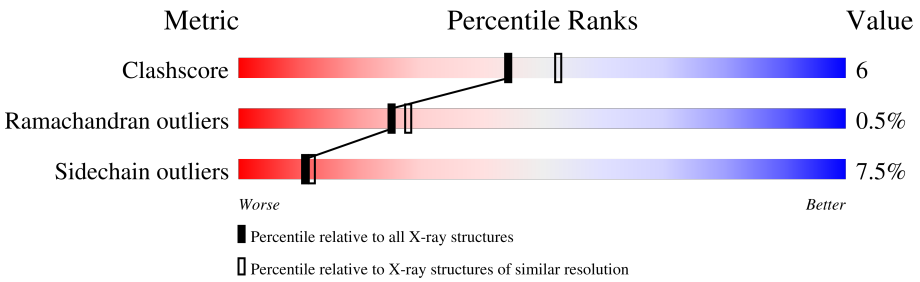
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.20 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))
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	450	72% 18% • 8%
1	B	450	76% 14% • 8%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7099 atoms, of which 1 is hydrogen 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 Interstitial collagenase.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	415	Total C N O S 3347 2157 564 614 12	30	0	0
1	B	416	Total C H N O S 3327 2146 1 563 606 11	1	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Ca 4 4	0	0
2	B	4	Total Ca 4 4	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

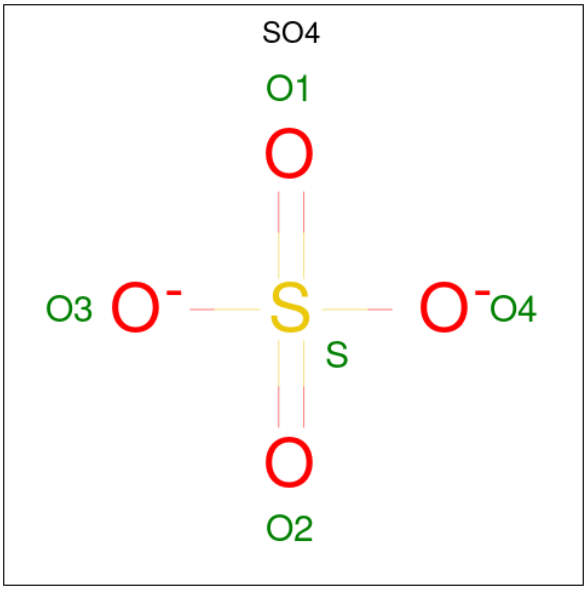
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

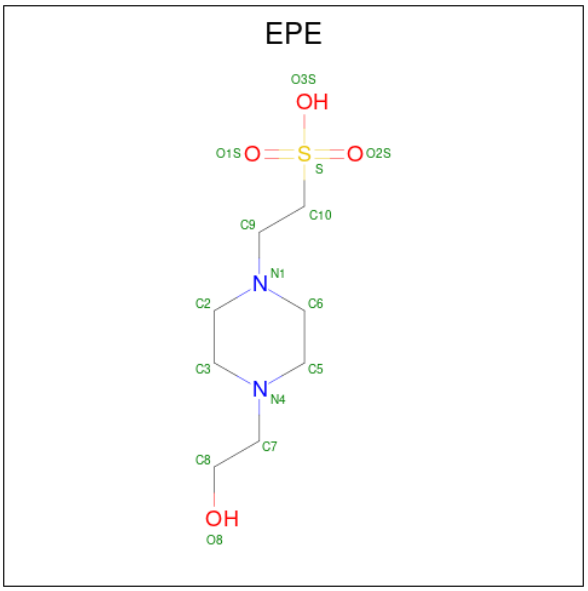
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	B	1	12	6	2	3	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	193	193	193	0	0
			Total	O		
8	B	179	179	179	0	0

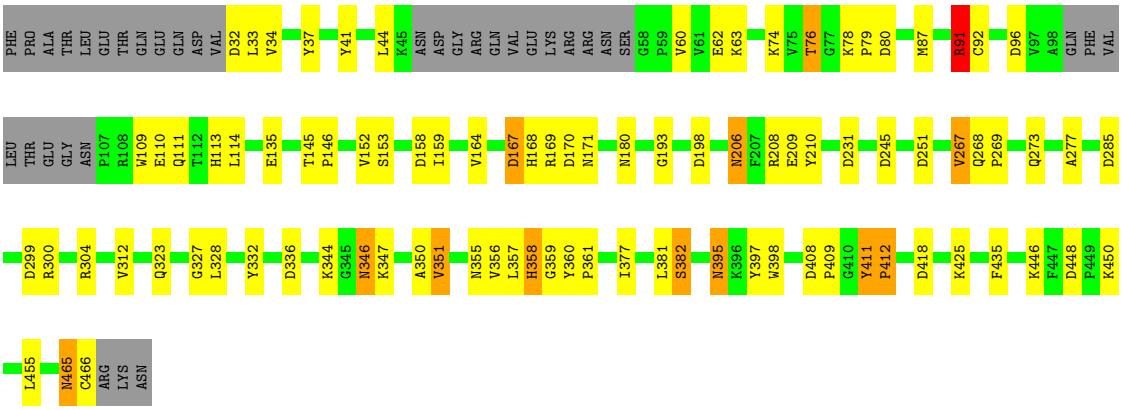
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

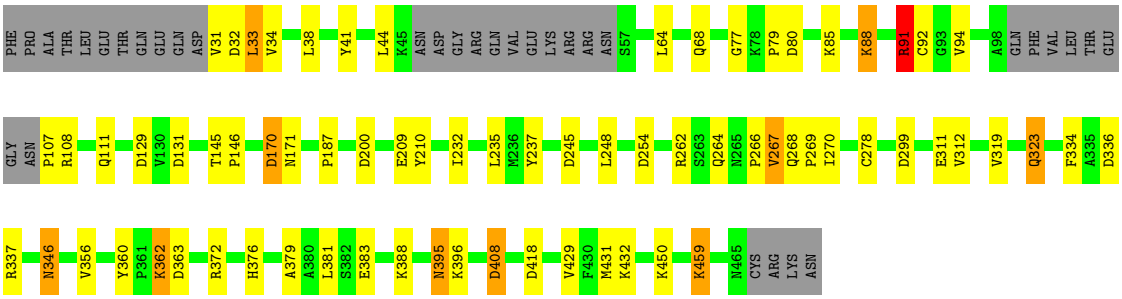
• Molecule 1: Interstitial collagenase

Chain A: 72% 18% • 8%



• Molecule 1: Interstitial collagenase

Chain B: 76% 14% • 8%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	142.75Å 142.75Å 295.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7099	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, CL, EPE, NA, 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	0.63	3/3452 (0.1%)	0.87	23/4679 (0.5%)
1	B	0.55	0/3431	0.80	13/4654 (0.3%)
All	All	0.59	3/6883 (0.0%)	0.83	36/9333 (0.4%)

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
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	CYS	C-O	14.47	1.50	1.23
1	A	358	HIS	C-N	-8.50	1.17	1.33
1	A	450	LYS	CA-CB	8.22	1.72	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	HIS	O-C-N	-14.84	97.97	123.20
1	A	465	ASN	N-CA-CB	8.81	126.46	110.60
1	A	355	ASN	CB-CA-C	-8.21	93.97	110.40
1	A	91	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	A	91	ARG	NE-CZ-NH2	7.99	124.30	120.30
1	A	411	TYR	N-CA-C	7.98	132.55	111.00
1	B	91	ARG	NE-CZ-NH1	-7.05	116.78	120.30
1	B	91	ARG	NE-CZ-NH2	6.74	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	418	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	465	ASN	CA-CB-CG	6.27	127.19	113.40
1	B	254	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	170	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	129	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	418	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	465	ASN	CB-CA-C	5.93	122.26	110.40
1	B	245	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	198	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	167	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	336	ASP	CB-CG-OD2	5.64	123.37	118.30
1	B	336	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	158	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	96	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	200	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	251	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	448	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	408	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	80	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	412	PRO	N-CA-C	-5.47	97.88	112.10
1	B	299	ASP	CB-CG-OD2	5.30	123.08	118.30
1	A	359	GLY	C-N-CA	5.30	134.96	121.70
1	A	408	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	299	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	358	HIS	CA-C-N	5.19	126.58	116.20
1	A	245	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	131	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	231	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	358	HIS	Mainchain

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	3347	0	3159	39	0
1	B	3326	1	3123	38	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	5	0	0	0	0
6	B	20	0	0	0	0
7	B	12	0	12	1	0
8	A	193	0	0	7	1
8	B	179	0	0	4	0
All	All	7098	1	6294	76	1

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 6.

All (76) 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:B:31:VAL:HG12	1:B:33:LEU:H	1.14	1.09
1:A:114:LEU:HD21	8:A:1071:HOH:O	1.72	0.89
1:B:323:GLN:HG2	1:B:356:VAL:HG21	1.58	0.85
1:A:300:ARG:NH2	8:A:1048:HOH:O	1.94	0.81
1:B:31:VAL:HG12	1:B:33:LEU:N	1.96	0.79
1:B:278:CYS:SG	8:B:1078:HOH:O	2.40	0.78
1:A:164:VAL:HG21	1:A:168:HIS:CD2	2.24	0.73
1:B:68:GLN:HE22	1:B:77:GLY:H	1.38	0.70
1:B:31:VAL:CG1	1:B:32:ASP:N	2.55	0.69
1:A:109:TRP:HB3	8:A:1071:HOH:O	1.92	0.69
1:B:395:ASN:HD22	1:B:395:ASN:H	1.40	0.69
1:B:107:PRO:O	1:B:187:PRO:HB2	1.93	0.67
1:B:31:VAL:HG12	1:B:32:ASP:N	2.10	0.67
1:A:113:HIS:ND1	8:A:1063:HOH:O	2.27	0.66
1:B:323:GLN:CG	1:B:356:VAL:HG21	2.27	0.65
1:B:85:LYS:HG3	1:B:88:LYS:NZ	2.12	0.64
1:A:395:ASN:H	1:A:395:ASN:HD22	1.47	0.62
1:A:114:LEU:CD2	8:A:1071:HOH:O	2.40	0.62
1:A:91:ARG:HD3	1:A:92:CYS:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:HD3	1:B:92:CYS:O	2.01	0.59
1:A:435:PHE:CD2	1:A:446:LYS:NZ	2.72	0.58
1:A:41:TYR:CZ	1:A:91:ARG:HD2	2.38	0.58
1:B:262:ARG:HD3	8:B:917:HOH:O	2.05	0.56
1:A:206:ASN:C	1:A:206:ASN:HD22	2.09	0.56
1:A:346:ASN:HD21	1:A:347:LYS:HE3	1.72	0.55
1:B:381:LEU:HD12	1:B:431:MET:HB2	1.89	0.54
1:A:44:LEU:HD21	1:A:60:VAL:HG22	1.90	0.54
1:B:34:VAL:HG21	1:B:79:PRO:HB3	1.90	0.54
1:A:409:PRO:O	8:A:923:HOH:O	2.19	0.54
1:B:346:ASN:HD22	1:B:346:ASN:C	2.11	0.54
1:A:346:ASN:HD22	1:A:347:LYS:HG3	1.72	0.53
1:B:395:ASN:HD22	1:B:395:ASN:N	2.03	0.53
1:B:41:TYR:CZ	1:B:91:ARG:HD2	2.44	0.53
1:B:360:TYR:CE1	1:B:362:LYS:HD3	2.43	0.52
1:A:327:GLY:O	1:A:344:LYS:HD3	2.09	0.52
1:A:332:TYR:CD2	1:A:382:SER:HB2	2.46	0.50
1:A:395:ASN:HD22	1:A:395:ASN:N	2.09	0.50
1:B:379:ALA:HB1	1:B:429:VAL:HG12	1.93	0.50
1:A:206:ASN:ND2	1:A:208:ARG:H	2.10	0.50
1:B:88:LYS:NZ	8:B:1089:HOH:O	2.40	0.48
1:A:145:THR:HB	1:A:146:PRO:HD2	1.96	0.48
1:A:170:ASP:O	1:A:171:ASN:HB2	2.14	0.48
1:B:85:LYS:HG3	1:B:88:LYS:HZ2	1.78	0.48
1:A:346:ASN:HD22	1:A:346:ASN:C	2.17	0.47
1:B:170:ASP:O	1:B:171:ASN:HB2	2.14	0.47
1:A:398:TRP:CH2	1:A:412:PRO:HG3	2.51	0.46
1:A:111:GLN:HE22	1:B:396:LYS:NZ	2.13	0.46
1:A:267:VAL:HG23	1:A:269:PRO:HD3	1.97	0.46
1:A:346:ASN:ND2	1:A:347:LYS:HG3	2.31	0.46
1:B:459:LYS:NZ	8:B:1035:HOH:O	2.39	0.45
1:B:360:TYR:CD1	1:B:362:LYS:HD3	2.52	0.45
1:A:76:THR:HG23	1:A:78:LYS:H	1.82	0.44
1:B:388:LYS:NZ	1:B:408:ASP:OD2	2.38	0.44
1:A:350:ALA:HB3	1:A:360:TYR:CE1	2.53	0.44
1:A:273:GLN:HG2	8:A:977:HOH:O	2.17	0.43
1:A:285:ASP:HB3	1:A:328:LEU:O	2.18	0.43
1:B:232:ILE:HA	1:B:237:TYR:CD1	2.54	0.43
1:A:277:ALA:HB2	1:A:312:VAL:HG11	2.00	0.43
1:A:397:TYR:O	1:A:411:TYR:O	2.37	0.43
1:B:383:GLU:HA	1:B:431:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:CG2	1:A:356:VAL:HG22	2.50	0.42
1:A:37:TYR:CE1	1:A:87:MET:HA	2.54	0.42
1:A:209:GLU:HA	1:A:210:TYR:HA	1.86	0.42
1:A:34:VAL:HG21	1:A:79:PRO:HB3	2.02	0.42
1:A:360:TYR:HA	1:A:361:PRO:C	2.40	0.42
1:B:94:VAL:HG13	7:B:600:EPE:H101	2.02	0.42
1:B:209:GLU:HA	1:B:210:TYR:HA	1.87	0.42
1:B:145:THR:HB	1:B:146:PRO:CD	2.50	0.41
1:A:159:ILE:HG23	1:A:193:GLY:O	2.20	0.41
1:A:145:THR:HB	1:A:146:PRO:CD	2.50	0.41
1:B:235:LEU:HD12	1:B:248:LEU:HD23	2.02	0.41
1:B:334:PHE:CE1	1:B:337:ARG:HD2	2.56	0.41
1:B:266:PRO:C	1:B:267:VAL:HG23	2.41	0.41
1:B:31:VAL:HG13	1:B:32:ASP:H	1.86	0.40
1:B:395:ASN:H	1:B:395:ASN:ND2	2.13	0.40
1:B:85:LYS:O	1:B:88:LYS:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1074:HOH:O	8:A:1074:HOH:O[15_545]	1.62	0.58

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	409/450 (91%)	395 (97%)	13 (3%)	1 (0%)	44 52
1	B	410/450 (91%)	399 (97%)	8 (2%)	3 (1%)	19 19
All	All	819/900 (91%)	794 (97%)	21 (3%)	4 (0%)	25 28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	PRO
1	B	268	GLN
1	A	169	ARG
1	B	267	VAL

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	350/389 (90%)	321 (92%)	29 (8%)	9 9
1	B	343/389 (88%)	320 (93%)	23 (7%)	13 15
All	All	693/778 (89%)	641 (92%)	52 (8%)	11 12

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	33	LEU
1	A	62	GLU
1	A	63	LYS
1	A	74	LYS
1	A	76	THR
1	A	80	ASP
1	A	91	ARG
1	A	110	GLU
1	A	135	GLU
1	A	152	VAL
1	A	153	SER
1	A	167	ASP
1	A	180	ASN
1	A	206	ASN
1	A	267	VAL
1	A	268	GLN
1	A	304	ARG
1	A	323	GLN

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Mol	Chain	Res	Type
1	A	346	ASN
1	A	351	VAL
1	A	357	LEU
1	A	377	ILE
1	A	381	LEU
1	A	382	SER
1	A	395	ASN
1	A	425	LYS
1	A	455	LEU
1	A	465	ASN
1	B	33	LEU
1	B	38	LEU
1	B	44	LEU
1	B	64	LEU
1	B	88	LYS
1	B	91	ARG
1	B	108	ARG
1	B	111	GLN
1	B	264	GLN
1	B	270	ILE
1	B	311	GLU
1	B	312	VAL
1	B	319	VAL
1	B	323	GLN
1	B	346	ASN
1	B	362	LYS
1	B	363	ASP
1	B	372	ARG
1	B	376	HIS
1	B	395	ASN
1	B	432	LYS
1	B	450	LYS
1	B	459	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	111	GLN
1	A	113	HIS
1	A	180	ASN
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	268	GLN
1	A	323	GLN
1	A	346	ASN
1	A	395	ASN
1	B	68	GLN
1	B	111	GLN
1	B	132	HIS
1	B	143	ASN
1	B	247	GLN
1	B	265	ASN
1	B	326	ASN
1	B	346	ASN
1	B	395	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)

Of 22 ligands modelled in this entry, 16 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
6	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.12	0
7	EPE	B	600	-	12,12,15	1.15	1 (8%)	15,16,20	1.71	3 (20%)
6	SO4	B	500	-	4,4,4	0.23	0	6,6,6	0.05	0
6	SO4	A	801	-	4,4,4	0.27	0	6,6,6	0.21	0
6	SO4	B	504	-	4,4,4	0.24	0	6,6,6	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EPE	B	600	-	-	1/6/14/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	600	EPE	C10-S	3.60	1.82	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	600	EPE	O1S-S-C10	3.81	112.49	106.73
7	B	600	EPE	C5-N4-C3	3.73	120.93	110.40
7	B	600	EPE	O2S-S-C10	2.54	110.57	106.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	600	EPE	S-C10-C9-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	600	EPE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	358:HIS	C	359:GLY	N	1.17

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.