Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2016 – 05:55 PM EST

PDB ID	:	1GTL
Title	:	The thermostable serine-carboxyl type proteinase, kumamolisin (KSCP) - complex with Ac-Ile-Pro-Phe-cho
Authors	:	Comellas-Bigler, M.; Fuentes-Prior, P.; Maskos, K.; Huber, R.; Oyama, H.; Uchida, K.; Dunn, B.M.; Oda, K.; Bode, W.
Deposited on	:	2002-01-16
Resolution	:	2.80 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 ⓘ symbol.

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

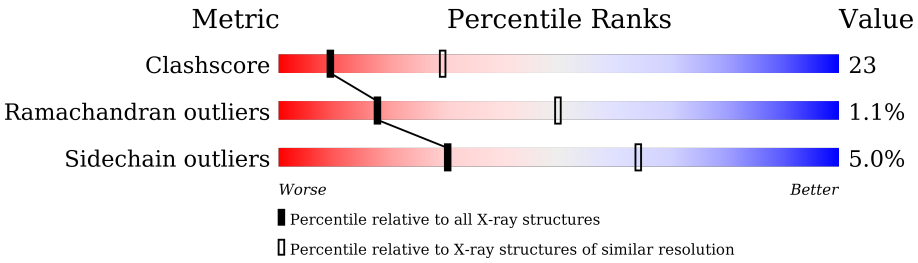
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	357	59% 38% .
1	2	357	62% 35% .
2	3	4	50% 50%
2	4	4	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5407 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 KUMAMOLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	357	Total	C	N	O	S	43	0	0
			2563	1612	434	513	4			
1	2	357	Total	C	N	O	S	50	0	0
			2563	1612	434	513	4			

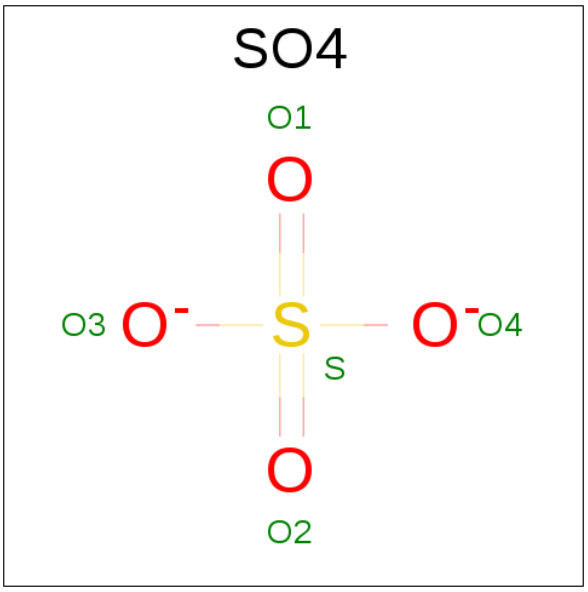
- Molecule 2 is a protein called ALDEHYDE INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	3	4	Total	C	N	O	0	0	0
			29	22	3	4			
2	4	4	Total	C	N	O	0	0	0
			29	22	3	4			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	2	1	Total	Ca	0	0
			1	1		
3	1	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1	1	Total O S 5 4 1	0	0
4	2	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1	107	Total O 107 107	0	0
5	2	102	Total O 102 102	0	0
5	3	1	Total O 1 1	0	0
5	4	1	Total O 1 1	0	0

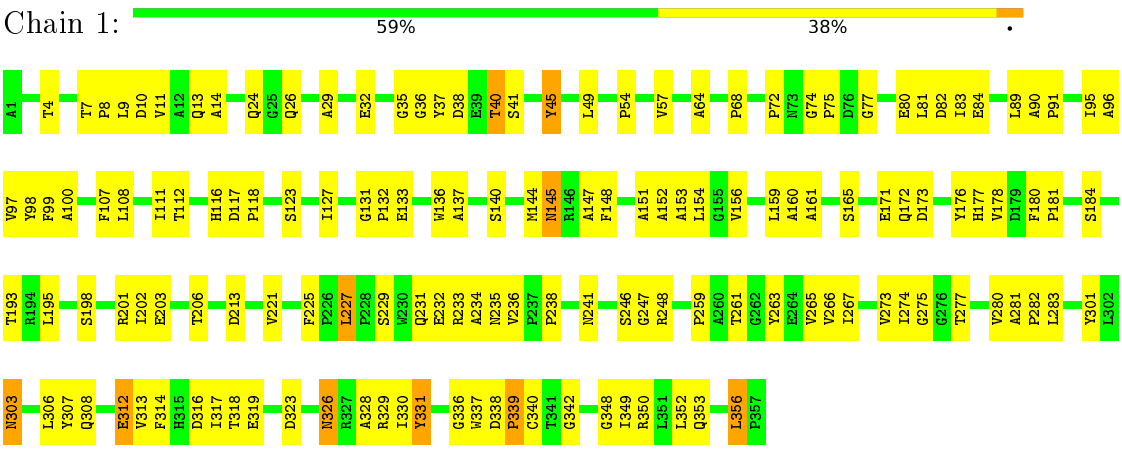
3 Residue-property plots (i)

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.

Note EDS was not executed.

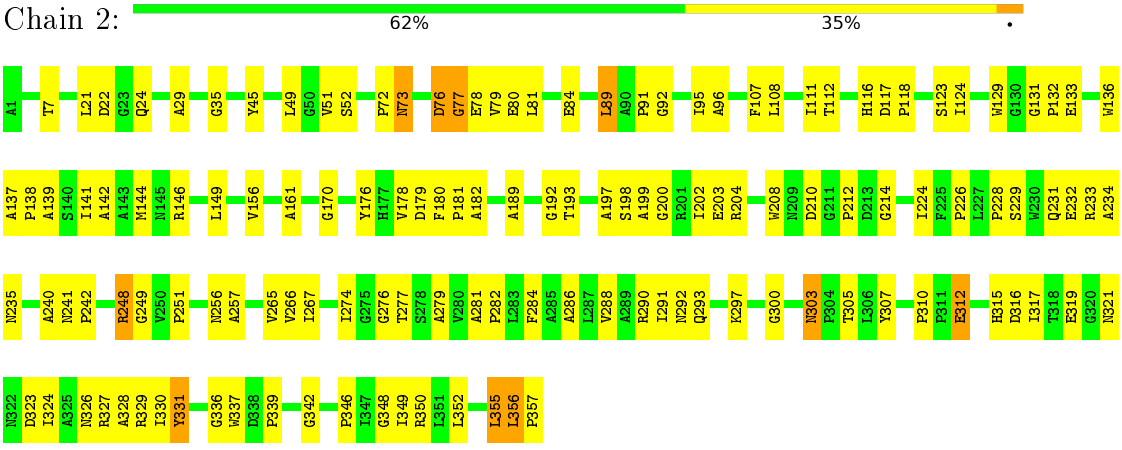
- Molecule 1: KUMAMOLYSIN

Chain 1:



- Molecule 1: KUMAMOLYSIN

Chain 2:



- Molecule 2: ALDEHYDE INHIBITOR

Chain 3:

- Molecule 2: ALDEHYDE INHIBITOR

Chain 4: 

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.03Å 78.30Å 73.17Å 90.00° 98.45° 90.00°	Depositor
Resolution (Å)	12.00 – 2.80	Depositor
% Data completeness (in resolution range)	90.1 (12.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.197 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5407	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1	0.47	0/2628	0.73	2/3611 (0.1%)
1	2	0.49	0/2628	0.73	1/3611 (0.0%)
2	3	1.61	0/16	2.82	2/22 (9.1%)
2	4	1.48	0/16	2.67	1/22 (4.5%)
All	All	0.49	0/5288	0.76	6/7266 (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
1	1	0	2
1	2	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	356	LEU	CA-CB-CG	6.28	129.75	115.30
2	4	2	ILE	O-C-N	-5.23	111.16	121.10
2	3	2	ILE	O-C-N	-5.19	111.23	121.10
2	3	3	PRO	CA-N-CD	-5.19	104.24	111.50
1	2	7	THR	N-CA-C	-5.09	97.24	111.00
1	1	7	THR	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	331	TYR	Sidechain
1	1	45	TYR	Sidechain
1	2	331	TYR	Sidechain

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	1	2563	0	2462	117	0
1	2	2563	0	2462	115	0
2	3	29	0	31	0	0
2	4	29	0	31	1	0
3	1	1	0	0	0	0
3	2	1	0	0	0	0
4	1	5	0	0	1	0
4	2	5	0	0	1	0
5	1	107	0	0	14	0
5	2	102	0	0	11	0
5	3	1	0	0	0	0
5	4	1	0	0	0	0
All	All	5407	0	4986	228	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 23.

All (228) 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)
1:1:353:GLN:HG3	5:1:2106:HOH:O	1.47	1.15
1:2:176:TYR:H	1:2:241:ASN:HD21	1.14	0.94
1:1:326:ASN:HD22	1:1:328:ALA:H	1.15	0.94
1:2:356:LEU:HD23	1:2:357:PRO:HD2	1.56	0.86
1:1:353:GLN:CG	5:1:2106:HOH:O	2.14	0.85
1:1:312:GLU:HG2	1:1:350:ARG:HD3	1.57	0.84
1:1:83:ILE:HD11	1:1:97:VAL:HG21	1.61	0.83
1:2:329:ARG:HD2	5:2:2094:HOH:O	1.77	0.83
1:1:45:TYR:CD1	1:1:84:GLU:HG2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:72:PRO:HA	1:2:267:ILE:HG22	1.61	0.80
1:2:179:ASP:O	1:2:182:ALA:HB3	1.81	0.80
1:1:203:GLU:HG2	1:2:226:PRO:HB3	1.64	0.79
1:1:24:GLN:HB2	5:1:2007:HOH:O	1.81	0.79
1:2:326:ASN:HB3	1:2:328:ALA:H	1.49	0.77
1:1:77:GLY:HA2	1:1:267:ILE:HD13	1.66	0.77
1:2:49:LEU:HB2	1:2:51:VAL:HG22	1.65	0.76
1:1:312:GLU:O	1:1:350:ARG:HD3	1.86	0.74
1:1:331:TYR:O	1:1:340:CYS:SG	2.47	0.72
1:2:303:ASN:N	1:2:303:ASN:HD22	1.85	0.72
1:1:193:THR:HG21	1:1:317:ILE:HD13	1.70	0.72
1:1:108:LEU:O	1:1:112:THR:HG23	1.90	0.71
1:2:303:ASN:HD22	1:2:303:ASN:H	1.38	0.70
1:2:229:SER:HA	1:2:232:GLU:OE1	1.91	0.70
1:1:180:PHE:CG	1:1:181:PRO:HA	2.27	0.70
1:1:213:ASP:HA	5:1:2055:HOH:O	1.91	0.69
1:2:315:HIS:HE1	5:2:2057:HOH:O	1.75	0.69
1:2:331:TYR:HB3	1:2:339:PRO:HG2	1.75	0.68
1:1:238:PRO:O	5:1:2069:HOH:O	2.11	0.68
1:1:4:THR:HG22	1:2:224:ILE:HG23	1.75	0.68
1:1:326:ASN:HD22	1:1:328:ALA:N	1.88	0.67
1:1:148:PHE:O	1:1:151:ALA:HB3	1.94	0.67
1:1:329:ARG:HD2	5:1:2096:HOH:O	1.93	0.67
1:2:229:SER:O	1:2:232:GLU:HG3	1.94	0.67
1:2:129:TRP:CZ3	2:4:3:PRO:HD3	2.30	0.66
1:1:9:LEU:HD12	1:1:49:LEU:HD22	1.79	0.65
1:1:161:ALA:HB1	1:1:277:THR:CB	2.26	0.65
1:1:227:LEU:CD2	5:1:2074:HOH:O	2.45	0.65
1:1:161:ALA:HB1	1:1:277:THR:HB	1.77	0.65
1:2:116:HIS:O	1:2:118:PRO:HD3	1.97	0.65
1:2:72:PRO:HA	1:2:267:ILE:CG2	2.28	0.64
1:2:24:GLN:HB3	1:2:293:GLN:NE2	2.13	0.64
1:1:331:TYR:HB3	1:1:339:PRO:HG2	1.80	0.64
1:1:13:GLN:HG3	5:2:2037:HOH:O	1.98	0.63
1:2:22:ASP:O	1:2:92:GLY:N	2.32	0.63
1:2:81:LEU:HD22	1:2:274:ILE:HG21	1.80	0.62
1:2:133:GLU:HG2	1:2:178:VAL:O	2.00	0.62
1:1:326:ASN:ND2	1:1:328:ALA:H	1.92	0.62
1:1:193:THR:HG21	1:1:317:ILE:CD1	2.30	0.62
1:2:80:GLU:O	1:2:84:GLU:HG3	1.99	0.61
1:2:312:GLU:H	1:2:312:GLU:CD	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:210:ASP:HB3	1:2:214:GLY:HA3	1.83	0.61
1:2:197:ALA:HA	1:2:203:GLU:OE1	2.00	0.61
1:2:337:TRP:HA	1:2:342:GLY:O	2.00	0.61
1:2:76:ASP:O	1:2:79:VAL:N	2.35	0.60
1:1:72:PRO:HA	1:1:267:ILE:HG22	1.83	0.60
1:2:193:THR:HG21	1:2:317:ILE:HD13	1.82	0.59
1:2:234:ALA:O	1:2:235:ASN:HB2	2.01	0.59
1:2:274:ILE:HD11	5:2:2020:HOH:O	2.03	0.59
1:2:310:PRO:HB2	1:2:312:GLU:OE2	2.02	0.59
1:2:323:ASP:OD1	1:2:326:ASN:HB2	2.02	0.59
1:2:77:GLY:HA2	1:2:267:ILE:HG12	1.84	0.58
1:1:312:GLU:HG2	1:1:312:GLU:O	2.04	0.58
1:2:303:ASN:ND2	1:2:303:ASN:H	2.02	0.58
1:1:274:ILE:HG22	1:1:275:GLY:N	2.19	0.57
1:2:180:PHE:CG	1:2:181:PRO:HA	2.39	0.57
1:1:349:ILE:HG23	1:1:350:ARG:N	2.19	0.57
1:1:303:ASN:HD22	1:1:303:ASN:N	2.01	0.57
1:1:32:GLU:O	1:1:99:PHE:HA	2.04	0.57
1:1:273:VAL:HG23	1:2:139:ALA:HB2	1.86	0.56
1:1:152:ALA:C	1:1:154:LEU:H	2.08	0.56
1:1:180:PHE:CD2	1:1:181:PRO:HA	2.41	0.56
1:1:108:LEU:HD13	1:1:144:MET:HG3	1.88	0.56
1:1:326:ASN:ND2	1:1:328:ALA:HB3	2.21	0.55
1:1:176:TYR:N	1:1:241:ASN:HD21	2.03	0.55
1:2:193:THR:HG21	1:2:317:ILE:CD1	2.37	0.55
1:1:161:ALA:HB1	1:1:277:THR:OG1	2.06	0.55
1:2:136:TRP:HB2	1:2:141:ILE:HD11	1.89	0.54
1:1:301:TYR:CE2	1:1:303:ASN:HB2	2.42	0.54
1:1:323:ASP:OD1	1:1:326:ASN:ND2	2.41	0.54
1:2:189:ALA:O	1:2:251:PRO:HB2	2.07	0.54
1:1:227:LEU:HG	5:1:2074:HOH:O	2.07	0.54
1:1:281:ALA:N	1:1:282:PRO:HD2	2.22	0.54
1:1:349:ILE:HG23	1:1:350:ARG:H	1.73	0.54
1:2:21:LEU:O	1:2:290:ARG:HD3	2.07	0.54
1:2:22:ASP:O	1:2:92:GLY:CA	2.56	0.54
1:2:77:GLY:HA2	1:2:267:ILE:CG1	2.39	0.53
1:2:266:VAL:C	1:2:267:ILE:HD12	2.29	0.53
1:1:40:THR:HG22	1:1:41:SER:N	2.23	0.53
1:1:29:ALA:HB1	1:1:98:TYR:CE1	2.44	0.53
1:2:80:GLU:OE2	1:2:267:ILE:HA	2.09	0.53
1:1:231:GLN:HG3	1:1:307:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:108:LEU:O	1:2:112:THR:HG23	2.09	0.52
1:1:229:SER:HA	1:1:232:GLU:OE2	2.09	0.52
1:2:29:ALA:HA	1:2:96:ALA:O	2.10	0.52
1:2:305:THR:HG21	1:2:355:LEU:HD11	1.91	0.52
1:2:133:GLU:O	1:2:141:ILE:HD11	2.10	0.52
1:2:24:GLN:HB3	1:2:293:GLN:HE22	1.75	0.51
1:1:123:SER:O	1:1:156:VAL:HA	2.11	0.51
1:1:233:ARG:NH2	5:1:2062:HOH:O	2.41	0.51
1:2:161:ALA:HB1	1:2:277:THR:OG1	2.11	0.51
1:1:9:LEU:CD1	1:1:49:LEU:HD22	2.40	0.51
1:1:36:GLY:HA3	1:1:68:PRO:HD3	1.93	0.50
1:1:8:PRO:O	1:1:89:LEU:HD21	2.11	0.50
1:1:328:ALA:O	1:1:329:ARG:HB2	2.12	0.50
1:2:149:LEU:HD23	1:2:149:LEU:C	2.31	0.50
1:2:350:ARG:NH1	5:2:2099:HOH:O	2.44	0.50
1:1:145:ASN:ND2	1:1:184:SER:OG	2.45	0.49
1:1:95:ILE:HD13	1:1:95:ILE:N	2.27	0.49
1:1:111:ILE:HD13	1:1:148:PHE:CE1	2.47	0.49
1:1:316:ASP:C	1:1:316:ASP:OD1	2.51	0.49
1:1:64:ALA:HB3	1:1:100:ALA:HA	1.94	0.49
1:2:161:ALA:HB1	1:2:277:THR:CB	2.43	0.49
1:2:231:GLN:HG3	1:2:307:TYR:CE2	2.47	0.49
1:1:326:ASN:HB3	5:1:2094:HOH:O	2.12	0.49
1:1:159:LEU:N	1:1:159:LEU:HD12	2.27	0.49
1:1:57:VAL:HG22	1:1:95:ILE:O	2.13	0.49
1:2:108:LEU:CD1	1:2:144:MET:HG2	2.43	0.49
1:2:123:SER:O	1:2:156:VAL:HA	2.13	0.49
1:1:145:ASN:OD1	1:1:225:PHE:HE2	1.96	0.49
1:2:89:LEU:HB3	1:2:286:ALA:HB1	1.95	0.48
1:2:349:ILE:HG23	1:2:350:ARG:N	2.28	0.48
1:1:133:GLU:HG2	1:1:178:VAL:O	2.13	0.48
1:2:202:ILE:HD12	1:2:315:HIS:CD2	2.48	0.48
1:2:316:ASP:C	1:2:316:ASP:OD1	2.51	0.48
1:1:282:PRO:HD3	5:1:2030:HOH:O	2.13	0.48
1:1:127:ILE:O	1:1:160:ALA:HA	2.14	0.48
1:2:210:ASP:CB	1:2:214:GLY:HA3	2.44	0.48
1:1:326:ASN:HD21	1:1:328:ALA:HB3	1.78	0.47
1:2:176:TYR:HD1	1:2:241:ASN:ND2	2.12	0.47
1:2:267:ILE:HD12	1:2:267:ILE:N	2.30	0.47
1:1:132:PRO:O	1:1:136:TRP:CD1	2.67	0.47
1:1:227:LEU:HD21	5:1:2074:HOH:O	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:200:GLY:N	4:2:1359:SO4:O4	2.47	0.47
1:1:316:ASP:OD1	1:1:318:THR:HG22	2.15	0.47
1:1:229:SER:O	1:1:232:GLU:HG3	2.15	0.47
1:1:84:GLU:OE1	1:1:265:VAL:HB	2.15	0.47
1:2:124:ILE:CD1	1:2:288:VAL:HG12	2.45	0.47
1:1:37:TYR:O	1:1:37:TYR:CD1	2.68	0.47
1:2:279:ALA:O	1:2:282:PRO:HG2	2.15	0.47
1:1:236:VAL:HG21	5:1:2074:HOH:O	2.14	0.46
1:2:212:PRO:HG3	1:2:324:ILE:O	2.15	0.46
1:1:263:TYR:O	1:1:273:VAL:HA	2.16	0.46
1:2:180:PHE:CD2	1:2:181:PRO:HA	2.49	0.46
1:1:229:SER:HA	1:1:232:GLU:HG3	1.97	0.46
1:1:80:GLU:OE2	1:1:267:ILE:HA	2.16	0.46
1:2:108:LEU:HD13	1:2:144:MET:HG2	1.96	0.46
1:2:193:THR:O	1:2:256:ASN:HA	2.16	0.46
1:2:95:ILE:N	1:2:95:ILE:HD13	2.31	0.46
1:2:321:ASN:HB2	1:2:331:TYR:O	2.15	0.45
1:2:22:ASP:O	1:2:92:GLY:HA3	2.17	0.45
1:2:84:GLU:OE1	1:2:265:VAL:HB	2.16	0.45
1:2:330:ILE:HA	1:2:331:TYR:HA	1.70	0.45
1:1:176:TYR:H	1:1:241:ASN:HD21	1.64	0.45
1:1:274:ILE:CG2	1:1:275:GLY:N	2.79	0.45
1:1:313:VAL:HG12	1:1:313:VAL:O	2.15	0.45
1:1:176:TYR:HD1	1:1:241:ASN:ND2	2.14	0.45
1:2:300:GLY:HA3	5:2:2082:HOH:O	2.16	0.45
1:1:45:TYR:CD2	1:1:266:VAL:HG23	2.51	0.45
1:1:90:ALA:N	1:1:91:PRO:CD	2.80	0.45
1:2:176:TYR:H	1:2:241:ASN:ND2	1.97	0.45
1:1:337:TRP:HA	1:1:342:GLY:O	2.18	0.44
1:2:312:GLU:O	1:2:350:ARG:HD2	2.18	0.44
1:2:240:ALA:CB	1:2:330:ILE:HG21	2.47	0.44
1:2:161:ALA:HB1	1:2:277:THR:HB	1.98	0.44
1:1:35:GLY:HA3	1:1:75:PRO:HB2	1.99	0.44
1:1:137:ALA:O	1:1:140:SER:HB2	2.16	0.44
1:1:54:PRO:HB3	1:1:91:PRO:O	2.18	0.44
1:2:265:VAL:HG23	1:2:267:ILE:HD13	1.99	0.44
1:1:144:MET:O	1:1:147:ALA:HB3	2.17	0.44
1:2:124:ILE:HD11	1:2:288:VAL:HG12	1.99	0.44
1:2:198:SER:O	1:2:199:ALA:C	2.56	0.44
1:2:315:HIS:CE1	5:2:2057:HOH:O	2.57	0.44
1:2:323:ASP:OD2	1:2:326:ASN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:131:GLY:O	1:1:132:PRO:C	2.57	0.43
1:2:208:TRP:CH2	1:2:276:GLY:HA2	2.52	0.43
1:1:306:LEU:HD22	1:1:314:PHE:HZ	1.84	0.43
1:2:131:GLY:O	1:2:132:PRO:C	2.55	0.43
1:2:281:ALA:N	1:2:282:PRO:HD2	2.33	0.43
1:2:330:ILE:HG23	1:2:331:TYR:CD2	2.53	0.43
1:2:45:TYR:CE1	1:2:84:GLU:HB3	2.54	0.43
1:1:116:HIS:O	1:1:118:PRO:HD3	2.19	0.43
1:1:74:GLY:O	1:1:75:PRO:C	2.56	0.43
1:2:233:ARG:HH21	1:2:233:ARG:HG3	1.83	0.43
1:1:201:ARG:NH1	4:1:1359:SO4:O3	2.51	0.43
1:1:81:LEU:HG	1:1:82:ASP:N	2.34	0.43
1:1:206:THR:HG22	1:1:319:GLU:HB2	2.01	0.43
1:1:336:GLY:O	1:1:337:TRP:C	2.58	0.43
1:2:336:GLY:O	1:2:337:TRP:C	2.57	0.43
1:2:291:ILE:O	1:2:292:ASN:C	2.57	0.42
1:1:132:PRO:HB3	1:1:171:GLU:OE1	2.19	0.42
1:2:228:PRO:O	1:2:232:GLU:HG2	2.19	0.42
1:1:234:ALA:O	1:1:235:ASN:HB2	2.19	0.42
1:1:259:PRO:C	1:1:261:THR:H	2.23	0.42
1:1:195:LEU:HD11	1:1:202:ILE:HG12	2.01	0.42
1:1:72:PRO:HA	1:1:267:ILE:CG2	2.50	0.42
1:1:221:VAL:HG12	1:1:247:GLY:HA3	2.00	0.42
1:2:22:ASP:HB2	1:2:91:PRO:HG2	2.00	0.42
1:2:242:PRO:N	5:2:2075:HOH:O	2.51	0.42
1:1:45:TYR:HD2	1:1:266:VAL:HG23	1.84	0.42
1:2:117:ASP:HA	1:2:118:PRO:HD2	1.94	0.42
1:2:352:LEU:CD2	1:2:356:LEU:HD12	2.49	0.42
1:1:173:ASP:OD1	1:1:177:HIS:CE1	2.73	0.42
1:1:307:TYR:OH	1:1:337:TRP:NE1	2.53	0.42
1:2:170:GLY:N	5:2:2044:HOH:O	2.48	0.42
1:1:117:ASP:HA	5:1:2027:HOH:O	2.19	0.42
1:2:111:ILE:HG13	1:2:144:MET:CE	2.50	0.41
1:2:235:ASN:N	5:2:2071:HOH:O	2.52	0.41
1:2:284:PHE:CZ	1:2:346:PRO:HD2	2.54	0.41
1:2:356:LEU:HA	1:2:357:PRO:HD2	1.77	0.41
1:1:338:ASP:HB2	1:1:339:PRO:HD2	2.02	0.41
1:1:152:ALA:O	1:1:154:LEU:N	2.53	0.41
1:2:73:ASN:HD22	1:2:73:ASN:HA	1.46	0.41
1:1:11:VAL:O	1:1:14:ALA:HB3	2.21	0.41
1:2:192:GLY:HA3	1:2:257:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:281:ALA:HB3	1:2:282:PRO:CD	2.50	0.41
1:2:76:ASP:O	1:2:78:GLU:N	2.54	0.41
1:2:327:ARG:HH11	1:2:327:ARG:HG3	1.85	0.41
1:1:10:ASP:OD2	1:2:146:ARG:NH1	2.49	0.41
1:1:198:SER:OG	1:1:203:GLU:OE2	2.35	0.41
1:1:152:ALA:C	1:1:154:LEU:N	2.73	0.41
1:2:137:ALA:O	1:2:138:PRO:C	2.59	0.41
1:2:204:ARG:NH1	1:2:319:GLU:OE1	2.45	0.41
1:2:242:PRO:CD	5:2:2075:HOH:O	2.69	0.41
1:2:231:GLN:O	1:2:231:GLN:HG2	2.20	0.41
1:1:57:VAL:HG23	1:1:96:ALA:HA	2.02	0.40
1:2:248:ARG:HD3	1:2:249:GLY:O	2.22	0.40
1:1:280:VAL:HA	1:1:283:LEU:HB3	2.03	0.40
1:1:330:ILE:HA	1:1:331:TYR:HA	1.73	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	1	355/357 (99%)	322 (91%)	30 (8%)	3 (1%)	24 58
1	2	355/357 (99%)	315 (89%)	35 (10%)	5 (1%)	14 42
2	3	2/4 (50%)	2 (100%)	0	0	100 100
2	4	2/4 (50%)	2 (100%)	0	0	100 100
All	All	714/722 (99%)	641 (90%)	65 (9%)	8 (1%)	17 50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	153	ALA

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Mol	Chain	Res	Type
1	2	35	GLY
1	2	348	GLY
1	2	77	GLY
1	2	142	ALA
1	2	312	GLU
1	1	348	GLY
1	1	339	PRO

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	1	260/260 (100%)	244 (94%)	16 (6%)	23 54
1	2	260/260 (100%)	250 (96%)	10 (4%)	40 74
2	3	2/2 (100%)	2 (100%)	0	100 100
2	4	2/2 (100%)	2 (100%)	0	100 100
All	All	524/524 (100%)	498 (95%)	26 (5%)	30 64

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	26	GLN
1	1	38	ASP
1	1	40	THR
1	1	107	PHE
1	1	145	ASN
1	1	165	SER
1	1	172	GLN
1	1	227	LEU
1	1	246	SER
1	1	248	ARG
1	1	303	ASN
1	1	308	GLN
1	1	312	GLU
1	1	326	ASN

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Mol	Chain	Res	Type
1	1	352	LEU
1	1	356	LEU
1	2	52	SER
1	2	73	ASN
1	2	76	ASP
1	2	89	LEU
1	2	107	PHE
1	2	248	ARG
1	2	297	LYS
1	2	303	ASN
1	2	355	LEU
1	2	356	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	44	GLN
1	1	145	ASN
1	1	235	ASN
1	1	241	ASN
1	1	303	ASN
1	1	326	ASN
1	2	24	GLN
1	2	73	ASN
1	2	145	ASN
1	2	235	ASN
1	2	241	ASN
1	2	303	ASN
1	2	308	GLN
1	2	315	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	PHL	3	4	1,2	11,11,11	2.27	7 (63%)	10,13,13	2.06	2 (20%)
2	PHL	4	4	1,2	11,11,11	2.27	7 (63%)	10,13,13	1.95	1 (10%)

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
2	PHL	3	4	1,2	-	0/6/6/6	0/1/1/1
2	PHL	4	4	1,2	-	0/6/6/6	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	4	PHL	CD1-CG	2.12	1.43	1.38
2	3	4	PHL	CD1-CG	2.27	1.43	1.38
2	3	4	PHL	CB-CA	2.48	1.57	1.53
2	4	4	PHL	CE2-CD2	2.66	1.44	1.38
2	4	4	PHL	CB-CA	2.72	1.58	1.53
2	4	4	PHL	CZ-CE1	2.79	1.45	1.38
2	3	4	PHL	CZ-CE1	2.79	1.45	1.38
2	3	4	PHL	CE2-CD2	2.82	1.44	1.38
2	4	4	PHL	CZ-CE2	2.82	1.45	1.38
2	3	4	PHL	CZ-CE2	2.85	1.45	1.38
2	3	4	PHL	CE1-CD1	3.05	1.44	1.38
2	4	4	PHL	CD2-CG	3.08	1.45	1.38
2	4	4	PHL	CE1-CD1	3.08	1.44	1.38
2	3	4	PHL	CD2-CG	3.12	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3	4	PHL	CD2-CG-CD1	2.14	121.68	118.15
2	4	4	PHL	CG-CB-CA	5.23	122.86	113.25
2	3	4	PHL	CG-CB-CA	5.38	123.12	113.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	SO4	1	1359	-	4,4,4	0.43	0	6,6,6	0.22	0
4	SO4	2	1359	-	4,4,4	0.21	0	6,6,6	0.17	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
4	SO4	1	1359	-	-	0/0/0/0	0/0/0/0
4	SO4	2	1359	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	1	1359	SO4	1	0
4	2	1359	SO4	1	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.