



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:58 AM UTC

PDB ID : 1WPO / pdb_00001wpo
Title : HYDROLYTIC ENZYME HUMAN CYTOMEGALOVIRUS PROTEASE
Authors : Tong, L.
Deposited on : 1996-07-23
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

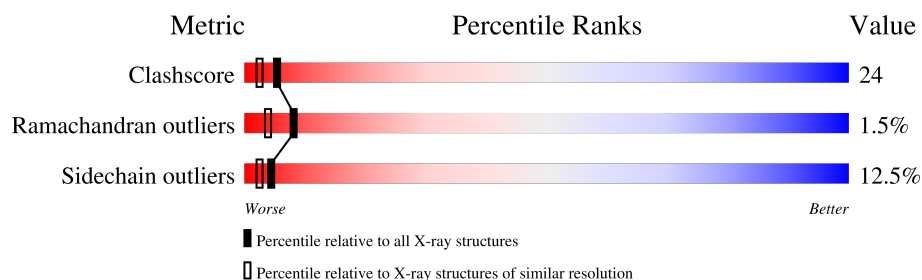
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	43% 29% 8% • 19%
1	B	256	50% 27% 5% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3539 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.

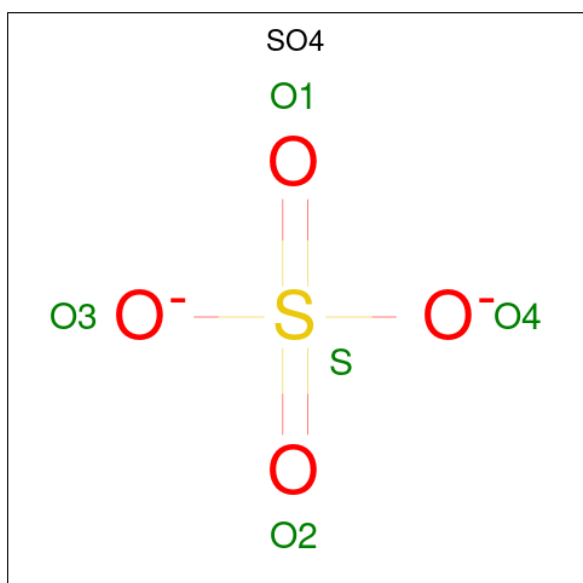
- Molecule 1 is a protein called HUMAN CYTOMEGALOVIRUS PROTEASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	Se	0	0	0
			1624	1025	297	296	3	3			
1	B	212	Total	C	N	O	S	Se	0	0	0
			1661	1048	301	306	3	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	MSE	MET	conflict	UNP P16753
A	181	MSE	THR	engineered mutation	UNP P16753
A	229	MSE	LEU	engineered mutation	UNP P16753
B	75	MSE	MET	modified residue	UNP P16753
B	181	MSE	THR	engineered mutation	UNP P16753
B	229	MSE	LEU	engineered mutation	UNP P16753

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

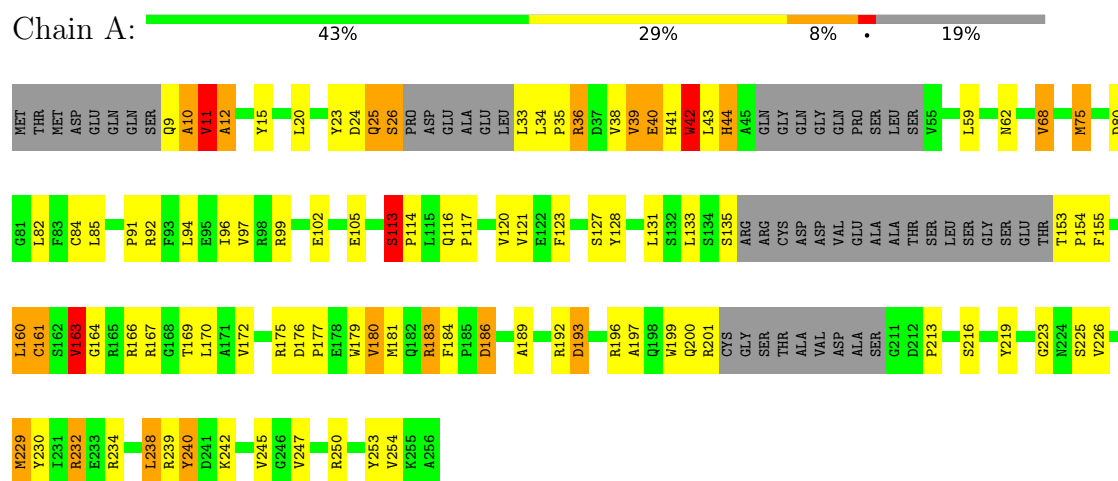
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		
3	B	136	Total	O	0	0
			136	136		

3 Residue-property plots

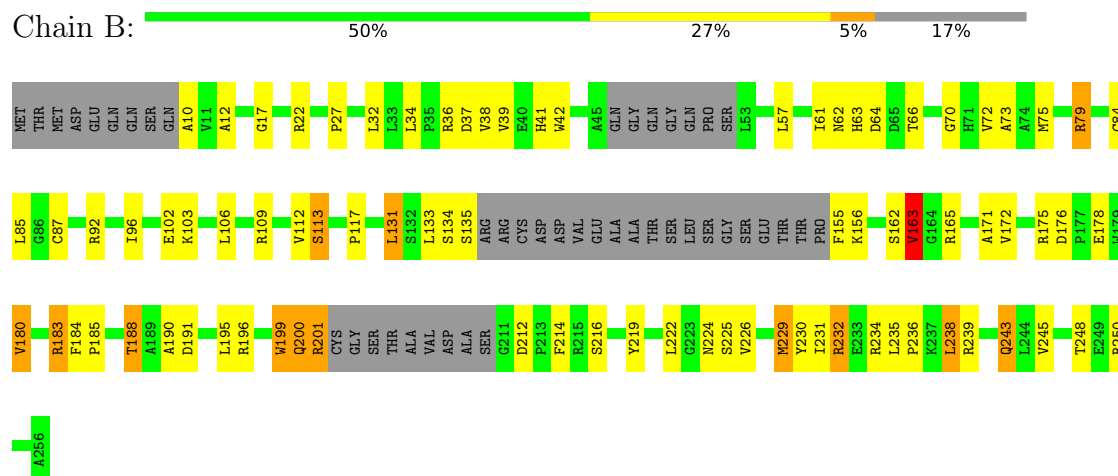
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: HUMAN CYTOMEGALOVIRUS PROTEASE



• Molecule 1: HUMAN CYTOMEGALOVIRUS PROTEASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.00Å 71.00Å 209.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.221 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3539	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: 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	0.60	0/1654	1.21	15/2232 (0.7%)
1	B	0.67	0/1692	1.15	8/2285 (0.4%)
All	All	0.64	0/3346	1.18	23/4517 (0.5%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	ALA	N-CA-C	-12.96	93.86	109.93
1	A	75	MSE	CG-SE-CE	12.61	126.66	98.92
1	A	12	ALA	N-CA-C	-11.00	95.13	110.31
1	A	232	ARG	N-CA-C	10.93	124.36	111.02
1	B	232	ARG	N-CA-C	10.03	121.91	110.97
1	B	229	MSE	CG-SE-CE	7.36	115.11	98.92
1	A	44	HIS	N-CA-C	7.32	120.31	111.82
1	A	41	HIS	N-CA-C	7.30	122.28	113.23
1	A	163	VAL	CB-CA-C	-7.10	101.93	111.80
1	A	181	MSE	CG-SE-CE	6.99	114.29	98.92
1	A	113	SER	N-CA-C	6.74	124.70	109.81
1	A	42	TRP	N-CA-C	-6.53	104.00	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	VAL	CB-CA-C	-6.39	102.92	111.80
1	B	231	ILE	N-CA-C	-6.36	99.12	108.54
1	B	41	HIS	N-CA-C	-6.31	104.48	111.36
1	B	113	SER	N-CA-C	6.25	123.62	109.81
1	B	75	MSE	CG-SE-CE	6.06	112.26	98.92
1	A	176	ASP	CA-C-N	5.37	125.44	119.32
1	A	176	ASP	C-N-CA	5.37	125.44	119.32
1	A	160	LEU	N-CA-C	-5.28	100.70	109.46
1	A	80	ASP	N-CA-C	5.23	119.82	113.38
1	A	240	TYR	N-CA-C	-5.20	105.69	111.36
1	A	229	MSE	CG-SE-CE	5.03	110.00	98.92

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	TYR	Sidechain
1	B	230	TYR	Sidechain

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	1624	0	1613	92	0
1	B	1661	0	1647	76	0
2	B	5	0	0	0	0
3	A	113	0	0	15	0
3	B	136	0	0	11	0
All	All	3539	0	3260	157	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 24.

All (157) 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:A:229:MSE:HE2	1:B:225:SER:HB2	1.67	0.75
1:A:226:VAL:HA	1:A:229:MSE:HE3	1.67	0.75
1:A:245:VAL:HG23	1:A:247:VAL:HG23	1.71	0.73
1:A:113:SER:HB3	1:A:114:PRO:HD3	1.71	0.71
1:B:73:ALA:HB1	1:B:199:TRP:HB2	1.74	0.70
1:A:99:ARG:HH11	1:A:99:ARG:HG2	1.58	0.69
1:A:39:VAL:O	1:A:43:LEU:HB3	1.93	0.67
3:A:653:HOH:O	1:B:229:MSE:SE	2.62	0.67
1:B:234:ARG:HD3	3:B:609:HOH:O	1.94	0.67
1:A:135:SER:HB2	1:A:155:PHE:CD1	2.29	0.67
1:A:225:SER:HB2	1:B:229:MSE:HE2	1.77	0.66
1:B:10:ALA:N	1:B:175:ARG:HH22	1.92	0.66
1:B:27:PRO:HD2	3:B:683:HOH:O	1.93	0.66
1:B:162:SER:HB2	1:B:234:ARG:HE	1.60	0.66
1:A:135:SER:HB2	1:A:155:PHE:HD1	1.60	0.66
1:B:163:VAL:HG22	1:B:234:ARG:HG3	1.79	0.65
1:B:165:ARG:HD2	3:B:842:HOH:O	1.97	0.65
1:B:36:ARG:NH1	1:B:79:ARG:HA	2.13	0.64
1:A:114:PRO:HA	3:A:751:HOH:O	1.98	0.64
1:B:163:VAL:HG13	1:B:238:LEU:HD13	1.80	0.63
1:A:33:LEU:O	1:A:35:PRO:HD3	1.99	0.63
1:A:10:ALA:HB1	1:A:120:VAL:HG21	1.80	0.62
1:B:196:ARG:HA	1:B:199:TRP:CE3	2.34	0.62
1:A:68:VAL:HG13	1:A:213:PRO:HB2	1.81	0.62
1:B:39:VAL:O	1:B:42:TRP:HB2	2.00	0.62
1:A:186:ASP:HB3	3:A:674:HOH:O	1.99	0.62
1:A:163:VAL:CG2	1:A:234:ARG:HG3	2.29	0.62
1:B:131:LEU:HD13	1:B:171:ALA:HB2	1.82	0.61
1:B:243:GLN:HG3	1:B:248:THR:HG21	1.83	0.61
1:A:225:SER:CB	1:B:229:MSE:HE2	2.30	0.60
1:B:172:VAL:HG11	1:B:183:ARG:HG2	1.83	0.60
1:B:195:LEU:HD13	3:B:738:HOH:O	2.02	0.60
1:B:200:GLN:O	1:B:201:ARG:HD3	2.02	0.60
1:A:25:GLN:HG2	1:A:167:ARG:HB2	1.84	0.59
1:A:116:GLN:HG2	1:A:117:PRO:HD2	1.85	0.58
1:A:201:ARG:HG3	3:A:810:HOH:O	2.03	0.58
1:A:62:ASN:ND2	1:A:161:CYS:HB3	2.19	0.58
1:B:163:VAL:CG2	1:B:234:ARG:HG3	2.33	0.58
1:A:9:GLN:HB3	3:A:819:HOH:O	2.04	0.58
1:B:199:TRP:CG	1:B:199:TRP:O	2.57	0.57
1:A:23:TYR:HE2	3:A:849:HOH:O	1.86	0.57
1:A:232:ARG:NE	1:B:239:ARG:HH22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:VAL:HA	1:B:229:MSE:HE3	1.87	0.56
1:A:189:ALA:HA	1:A:192:ARG:NH1	2.20	0.56
1:A:82:LEU:HD11	3:A:661:HOH:O	2.06	0.56
1:B:188:THR:HG22	1:B:190:ALA:N	2.21	0.55
1:A:20:LEU:HD13	1:A:133:LEU:HD13	1.87	0.55
1:A:35:PRO:O	1:A:39:VAL:HG22	2.06	0.55
1:B:200:GLN:C	1:B:201:ARG:HD3	2.32	0.55
1:B:92:ARG:NH2	1:B:212:ASP:HB3	2.21	0.55
1:B:226:VAL:HG22	1:B:229:MSE:HE3	1.89	0.55
1:A:34:LEU:HD21	1:A:133:LEU:HD23	1.88	0.54
1:A:25:GLN:NE2	1:A:240:TYR:HE2	2.04	0.54
1:B:188:THR:HG22	1:B:190:ALA:H	1.72	0.54
1:A:25:GLN:NE2	1:A:240:TYR:CE2	2.75	0.54
1:A:10:ALA:CB	1:A:120:VAL:HG21	2.38	0.54
1:A:163:VAL:HG22	1:A:234:ARG:HG3	1.89	0.54
1:A:36:ARG:HG3	1:A:40:GLU:OE2	2.08	0.53
1:A:26:SER:HB3	3:A:800:HOH:O	2.07	0.53
1:B:37:ASP:HB2	3:B:726:HOH:O	2.09	0.53
1:B:64:ASP:OD1	1:B:66:THR:HG22	2.08	0.53
1:A:120:VAL:HG23	3:A:782:HOH:O	2.09	0.52
1:B:133:LEU:O	1:B:134:SER:HB3	2.10	0.52
1:B:201:ARG:HH11	1:B:201:ARG:HG2	1.75	0.52
1:B:188:THR:HG23	3:B:631:HOH:O	2.10	0.52
1:B:57:LEU:HD23	1:B:72:VAL:HG21	1.91	0.51
1:A:163:VAL:HG21	1:A:234:ARG:HG3	1.93	0.51
1:B:72:VAL:HG13	1:B:84:CYS:SG	2.51	0.51
1:A:226:VAL:CA	1:A:229:MSE:HE3	2.37	0.51
1:B:201:ARG:HG2	1:B:201:ARG:NH1	2.26	0.51
1:A:9:GLN:O	1:A:10:ALA:HB2	2.11	0.51
1:A:36:ARG:O	1:A:40:GLU:HB2	2.11	0.51
1:A:250:ARG:HG2	1:A:250:ARG:HH11	1.76	0.50
1:A:170:LEU:HD22	1:A:242:LYS:HG2	1.93	0.50
1:B:34:LEU:HB2	3:B:791:HOH:O	2.11	0.50
1:A:44:HIS:HB2	3:A:755:HOH:O	2.11	0.50
1:A:193:ASP:HA	1:A:196:ARG:NH1	2.27	0.50
1:A:116:GLN:HG2	1:A:117:PRO:CD	2.41	0.49
1:B:162:SER:HB2	1:B:234:ARG:NE	2.27	0.49
1:A:25:GLN:OE1	1:A:25:GLN:HA	2.11	0.49
1:A:11:VAL:HG13	1:A:91:PRO:HA	1.94	0.49
1:A:163:VAL:HG13	1:A:238:LEU:HD22	1.95	0.49
1:B:184:PHE:HD2	1:B:245:VAL:CG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TYR:OH	1:A:39:VAL:HG21	2.13	0.49
1:B:183:ARG:O	1:B:250:ARG:HG3	2.12	0.49
1:B:224:ASN:HB3	3:B:765:HOH:O	2.13	0.49
1:A:197:ALA:O	1:A:201:ARG:HB3	2.12	0.48
1:A:68:VAL:CG1	1:A:213:PRO:HB2	2.42	0.48
1:A:11:VAL:HG22	3:A:705:HOH:O	2.14	0.48
1:A:25:GLN:HE21	1:A:240:TYR:HE2	1.60	0.48
1:A:239:ARG:HH21	1:B:232:ARG:NE	2.12	0.48
1:A:10:ALA:HA	1:A:175:ARG:HH22	1.78	0.47
1:A:15:TYR:CD2	1:A:177:PRO:HG3	2.48	0.47
1:B:188:THR:HB	1:B:191:ASP:CG	2.38	0.47
1:A:121:VAL:HG11	1:A:253:TYR:CD2	2.49	0.47
1:A:232:ARG:NE	1:B:239:ARG:NH2	2.63	0.47
1:A:242:LYS:HD2	1:A:254:VAL:HG11	1.97	0.47
1:A:128:TYR:HA	1:A:161:CYS:O	2.15	0.47
1:B:199:TRP:O	1:B:200:GLN:CB	2.63	0.46
1:A:96:ILE:HG23	1:B:219:TYR:HE1	1.80	0.46
1:A:219:TYR:HE1	1:B:96:ILE:HG23	1.80	0.46
1:A:166:ARG:O	1:A:169:THR:HG22	2.16	0.46
1:A:219:TYR:CE1	1:B:96:ILE:HG23	2.51	0.46
1:A:99:ARG:HH11	1:A:99:ARG:CG	2.28	0.46
1:B:79:ARG:HD2	3:B:834:HOH:O	2.16	0.46
1:A:20:LEU:HD12	3:A:837:HOH:O	2.16	0.45
1:A:10:ALA:C	1:A:12:ALA:H	2.24	0.45
1:A:239:ARG:NH2	1:B:232:ARG:CZ	2.79	0.45
1:B:106:LEU:HA	1:B:109:ARG:HH21	1.81	0.45
1:A:179:TRP:O	1:A:183:ARG:HD2	2.16	0.45
1:B:199:TRP:O	1:B:199:TRP:CD1	2.69	0.45
1:A:184:PHE:HB3	1:A:186:ASP:OD1	2.17	0.45
1:A:180:VAL:O	1:A:183:ARG:HB2	2.16	0.45
1:B:17:GLY:HA2	1:B:84:CYS:O	2.17	0.45
1:A:223:GLY:O	1:A:226:VAL:HG12	2.16	0.45
1:A:166:ARG:HH11	1:A:166:ARG:HG2	1.80	0.44
1:B:214:PHE:CZ	1:B:216:SER:HB3	2.52	0.44
1:B:232:ARG:HG2	3:B:767:HOH:O	2.17	0.44
1:B:180:VAL:O	1:B:183:ARG:HB2	2.18	0.44
1:A:123:PHE:CE1	1:B:226:VAL:HG21	2.52	0.44
1:B:112:VAL:HG23	1:B:112:VAL:O	2.18	0.44
3:A:634:HOH:O	1:B:103:LYS:HE3	2.18	0.43
1:A:155:PHE:HE2	3:A:769:HOH:O	2.00	0.43
1:B:62:ASN:O	1:B:63:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASP:OD1	1:B:178:GLU:HB2	2.18	0.43
1:B:225:SER:O	1:B:229:MSE:HG3	2.18	0.43
1:B:188:THR:HG21	3:B:633:HOH:O	2.18	0.43
1:B:196:ARG:HA	1:B:199:TRP:CZ3	2.54	0.43
1:A:59:LEU:HD11	1:A:160:LEU:HD21	2.01	0.43
1:A:97:VAL:HG13	1:A:123:PHE:CD2	2.54	0.43
1:B:199:TRP:O	1:B:200:GLN:HB3	2.19	0.43
1:A:43:LEU:HD21	1:A:75:MSE:HB3	2.01	0.42
1:B:188:THR:HG22	1:B:191:ASP:H	1.85	0.42
1:B:64:ASP:CG	1:B:66:THR:HG22	2.45	0.42
1:B:70:GLY:HA3	1:B:87:CYS:O	2.19	0.42
1:B:133:LEU:HD11	1:B:155:PHE:CG	2.55	0.42
1:A:153:THR:N	1:A:154:PRO:CD	2.82	0.42
1:B:61:ILE:HG22	1:B:62:ASN:OD1	2.19	0.42
1:A:42:TRP:NE1	1:A:43:LEU:HB2	2.35	0.42
1:A:75:MSE:SE	3:A:661:HOH:O	2.87	0.42
1:B:183:ARG:O	1:B:185:PRO:HD3	2.20	0.42
1:B:188:THR:HB	1:B:191:ASP:OD2	2.19	0.42
1:A:25:GLN:NE2	1:A:240:TYR:OH	2.53	0.41
1:A:172:VAL:HG11	1:A:183:ARG:HG2	2.02	0.41
1:A:250:ARG:HG2	1:A:250:ARG:NH1	2.34	0.41
1:A:167:ARG:NE	1:A:167:ARG:HA	2.34	0.41
1:A:33:LEU:HA	1:A:166:ARG:HH22	1.85	0.41
1:A:164:GLY:HA3	1:A:169:THR:HG21	2.01	0.41
1:A:113:SER:CB	1:A:114:PRO:HD3	2.48	0.41
1:A:92:ARG:NH1	1:A:216:SER:O	2.54	0.41
1:B:176:ASP:O	1:B:180:VAL:HG13	2.21	0.41
1:A:166:ARG:HG2	1:A:166:ARG:NH1	2.36	0.40
1:B:22:ARG:HA	1:B:22:ARG:HD2	1.74	0.40
1:B:188:THR:CG2	1:B:190:ALA:H	2.33	0.40
1:A:34:LEU:HD13	1:A:166:ARG:NH2	2.36	0.40
1:A:35:PRO:HD2	1:A:38:VAL:CG2	2.51	0.40
1:A:163:VAL:HG22	1:A:234:ARG:CG	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	197/256 (77%)	184 (93%)	9 (5%)	4 (2%)	6	2
1	B	204/256 (80%)	190 (93%)	12 (6%)	2 (1%)	12	8
All	All	401/512 (78%)	374 (93%)	21 (5%)	6 (2%)	8	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ALA
1	A	113	SER
1	B	113	SER
1	B	200	GLN
1	A	200	GLN
1	A	11	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	174/211 (82%)	150 (86%)	24 (14%)	3	2
1	B	178/211 (84%)	158 (89%)	20 (11%)	6	3
All	All	352/422 (83%)	308 (88%)	44 (12%)	4	2

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	24	ASP
1	A	25	GLN
1	A	26	SER
1	A	36	ARG
1	A	39	VAL
1	A	40	GLU
1	A	42	TRP
1	A	68	VAL
1	A	84	CYS
1	A	85	LEU
1	A	94	LEU
1	A	102	GLU
1	A	105	GLU
1	A	127	SER
1	A	131	LEU
1	A	161	CYS
1	A	163	VAL
1	A	180	VAL
1	A	183	ARG
1	A	186	ASP
1	A	193	ASP
1	A	199	TRP
1	A	238	LEU
1	B	32	LEU
1	B	38	VAL
1	B	79	ARG
1	B	85	LEU
1	B	102	GLU
1	B	117	PRO
1	B	131	LEU
1	B	135	SER
1	B	156	LYS
1	B	163	VAL
1	B	180	VAL
1	B	183	ARG
1	B	188	THR
1	B	199	TRP
1	B	201	ARG
1	B	222	LEU
1	B	235	LEU
1	B	236	PRO
1	B	238	LEU

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Mol	Chain	Res	Type
1	B	243	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	71	HIS
1	A	182	GLN
1	B	25	GLN
1	B	41	HIS
1	B	243	GLN

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](#)

1 ligand is 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	SO4	B	561	-	4,4,4	0.80	0	6,6,6	0.87	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.

No monomer is involved in short contacts.

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

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.