



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:52 AM UTC

PDB ID : 1GQF / pdb_00001gqf
Title : Crystal structure of human procaspase-7
Authors : Riedl, S.; Bode, W.; Fuentes-Prior, P.
Deposited on : 2001-11-23
Resolution : 2.90 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

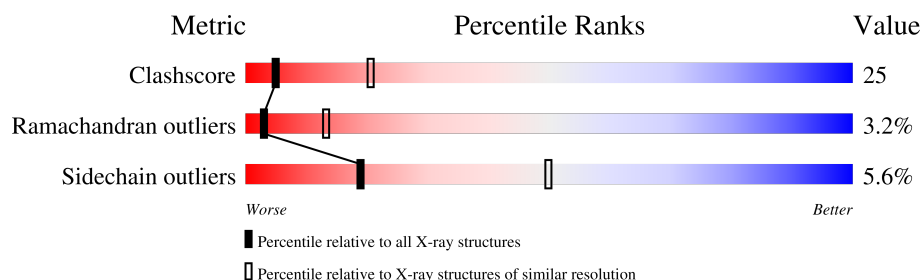
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	265	 58% 38% .
1	B	265	 60% 35% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4287 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 Caspase-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	564	0	0
			2126	1340	373	399	14			
1	B	265	Total	C	N	O	S	469	0	1
			2116	1335	369	398	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	ALA	CYS	engineered mutation	UNP P55210
A	402A	LEU	-	expression tag	UNP P55210
A	402B	GLU	-	expression tag	UNP P55210
A	402C	HIS	-	expression tag	UNP P55210
A	402D	HIS	-	expression tag	UNP P55210
A	402E	HIS	-	expression tag	UNP P55210
A	402F	HIS	-	expression tag	UNP P55210
A	402G	HIS	-	expression tag	UNP P55210
A	402H	HIS	-	expression tag	UNP P55210
B	285	ALA	CYS	engineered mutation	UNP P55210
B	402A	LEU	-	expression tag	UNP P55210
B	402B	GLU	-	expression tag	UNP P55210
B	402C	HIS	-	expression tag	UNP P55210
B	402D	HIS	-	expression tag	UNP P55210
B	402E	HIS	-	expression tag	UNP P55210
B	402F	HIS	-	expression tag	UNP P55210
B	402G	HIS	-	expression tag	UNP P55210
B	402H	HIS	-	expression tag	UNP P55210

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	13	Total	O	0	0
			13	13		

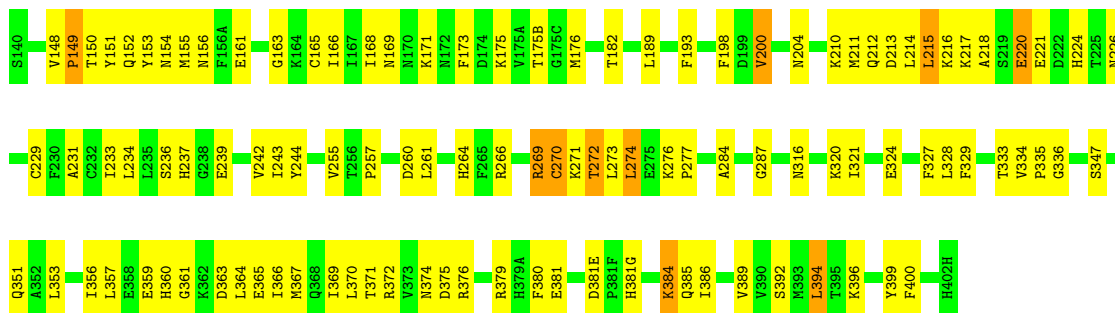
3 Residue-property plots

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.

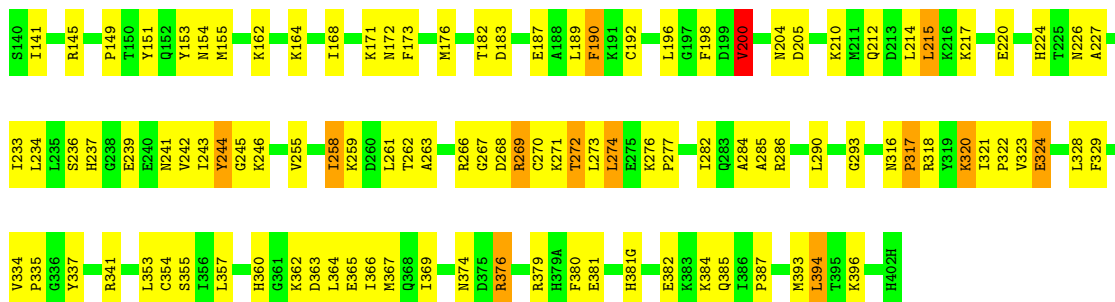
• Molecule 1: Caspase-7

Chain A: 



• Molecule 1: Caspase-7

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.21 Å 90.21 Å 183.02 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	21.73 – 2.90	Depositor
% Data completeness (in resolution range)	98.8 (21.73-2.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.268 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4287	wwPDB-VP
Average B, all atoms (Å ²)	79.0	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	0.51	2/2176 (0.1%)	0.87	9/2935 (0.3%)
1	B	0.53	2/2165 (0.1%)	0.89	7/2919 (0.2%)
All	All	0.52	4/4341 (0.1%)	0.88	16/5854 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	CYS	C-N	-7.93	1.23	1.34
1	B	270	CYS	C-N	-7.06	1.24	1.34
1	A	269	ARG	C-N	-6.87	1.25	1.33
1	B	269	ARG	C-N	-5.04	1.25	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	GLY	N-CA-C	-8.66	100.70	112.57
1	A	269	ARG	O-C-N	7.66	132.63	122.82
1	B	200	VAL	N-CA-C	6.80	118.46	109.21
1	A	148	VAL	C-N-CD	-6.80	105.64	120.60
1	A	150	THR	N-CA-C	-6.62	105.09	112.57
1	B	393	MET	N-CA-C	-6.23	103.83	112.30
1	A	269	ARG	CA-C-N	-6.21	113.56	122.93
1	A	269	ARG	C-N-CA	-6.21	113.56	122.93
1	A	381	GLU	N-CA-C	-5.54	106.42	114.12
1	A	221	GLU	N-CA-C	5.54	117.47	110.33
1	B	282	ILE	N-CA-C	5.45	115.74	108.11
1	B	269	ARG	O-C-N	5.43	129.81	122.59
1	B	337	TYR	CB-CA-C	-5.41	109.35	115.79
1	A	392	SER	N-CA-C	5.38	117.17	108.41
1	A	200	VAL	N-CA-C	5.21	116.78	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	TYR	N-CA-C	5.00	118.11	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2126	0	2062	81	0
1	B	2116	0	2049	78	0
2	A	5	0	0	0	0
2	B	20	0	0	1	0
3	A	7	0	0	0	0
3	B	13	0	0	0	0
All	All	4287	0	4111	159	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 25.

All (159) 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:168:ILE:HG21	1:A:211:MET:HE3	1.49	0.94
1:B:242:VAL:HG11	1:B:255:VAL:HB	1.59	0.83
1:B:242:VAL:CG1	1:B:255:VAL:HB	2.09	0.82
1:A:236:SER:HB3	1:A:243:ILE:HD11	1.61	0.81
1:B:271:LYS:HA	1:B:274:LEU:HD23	1.63	0.80
1:B:190:PHE:HD1	1:B:200:VAL:HG21	1.50	0.76
1:B:316:ASN:HD21	1:B:318:ARG:HD3	1.48	0.76
1:B:210:LYS:HD2	1:B:214:LEU:HD23	1.67	0.74
1:B:374:ASN:OD1	1:B:387:PRO:HG2	1.88	0.73
1:A:380:PHE:CD2	1:A:384:LYS:HA	2.24	0.73
1:B:189:LEU:HD13	1:B:233:ILE:HG21	1.70	0.72
1:A:353:LEU:O	1:A:357:LEU:HB2	1.90	0.71
1:A:171:LYS:HB2	1:A:182:THR:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LYS:HG3	1:B:321:ILE:HD12	1.74	0.70
1:A:214:LEU:HD12	1:A:215:LEU:N	2.09	0.67
1:A:149:PRO:HB2	1:A:151:TYR:HD1	1.60	0.66
1:B:171:LYS:HB2	1:B:182:THR:HG21	1.80	0.64
1:A:357:LEU:HD13	1:A:369:ILE:HG21	1.78	0.64
1:B:317:PRO:HB3	1:B:321:ILE:HD13	1.79	0.64
1:A:212:GLN:HE22	1:A:261:LEU:HD12	1.63	0.64
1:B:154:ASN:O	1:B:155:MET:HE2	1.97	0.64
1:A:154:ASN:HD21	1:A:156:ASN:HB3	1.62	0.64
1:A:189:LEU:HD13	1:A:233:ILE:HG21	1.80	0.63
1:B:154:ASN:C	1:B:155:MET:HE2	2.23	0.63
1:A:224:HIS:N	1:A:272:THR:OG1	2.30	0.62
1:A:176:MET:HE1	1:A:287:GLY:HA3	1.79	0.62
1:A:214:LEU:HD12	1:A:215:LEU:H	1.64	0.62
1:B:322:PRO:HD2	1:B:329:PHE:CZ	2.35	0.62
1:A:242:VAL:HG12	1:A:257:PRO:HA	1.82	0.61
1:A:216:LYS:HE2	1:A:220:GLU:OE2	2.01	0.61
1:A:321:ILE:HG12	1:A:321:ILE:O	2.00	0.60
1:A:169:ASN:HB3	1:A:204:ASN:ND2	2.17	0.60
1:B:258:ILE:HD11	1:B:320:LYS:HA	1.82	0.60
1:B:328:LEU:HD21	1:B:367:MET:HE1	1.84	0.60
1:A:347:SER:O	1:A:351:GLN:HG2	2.01	0.60
1:B:242:VAL:HG11	1:B:255:VAL:CB	2.31	0.59
1:A:360:HIS:HB3	1:A:364:LEU:HD22	1.85	0.59
1:B:172:ASN:O	1:B:246:LYS:HG3	2.03	0.59
1:A:154:ASN:ND2	1:A:156:ASN:H	2.01	0.58
1:A:149:PRO:HG2	1:A:152:GLN:HG3	1.84	0.58
1:B:239:GLU:HG3	1:B:286:ARG:NH1	2.19	0.57
1:A:365:GLU:OE2	1:A:366:ILE:HG22	2.04	0.57
1:B:239:GLU:HG3	1:B:286:ARG:HH12	1.70	0.57
1:B:360:HIS:HB3	1:B:364:LEU:HG	1.86	0.57
1:B:380:PHE:CD2	1:B:384:LYS:HA	2.41	0.56
1:B:321:ILE:HG23	1:B:329:PHE:CE2	2.41	0.55
1:A:153:TYR:CD2	1:A:396:LYS:HB2	2.42	0.55
1:B:258:ILE:HD13	1:B:259:LYS:H	1.71	0.54
1:A:271:LYS:HA	1:A:274:LEU:HD13	1.89	0.54
1:A:175:LYS:C	1:A:175(B):THR:H	2.15	0.54
1:A:212:GLN:NE2	1:A:261:LEU:HD12	2.23	0.54
1:A:328:LEU:HD21	1:A:367:MET:HE1	1.89	0.53
1:A:334:VAL:HG22	1:A:385:GLN:HB3	1.90	0.53
1:B:316:ASN:ND2	1:B:318:ARG:HD3	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:CYS:HB3	1:A:277:PRO:HG2	1.91	0.53
1:A:176:MET:HB3	1:A:237:HIS:CD2	2.44	0.53
1:A:324:GLU:HB2	1:A:327:PHE:CD1	2.43	0.53
1:B:365:GLU:OE1	1:B:366:ILE:HG22	2.10	0.53
1:B:149:PRO:HB2	1:B:151:TYR:HD2	1.74	0.52
1:B:176:MET:HB3	1:B:237:HIS:CD2	2.44	0.52
1:A:229:CYS:CB	1:A:277:PRO:HG2	2.39	0.52
1:B:266:ARG:NH2	1:B:324:GLU:HG3	2.24	0.52
1:A:154:ASN:HD21	1:A:156:ASN:CB	2.22	0.52
1:A:367:MET:HE1	1:A:389:VAL:HG11	1.91	0.51
1:A:171:LYS:HB2	1:A:182:THR:CG2	2.40	0.51
1:A:175(B):THR:HG22	1:A:176:MET:HG2	1.92	0.51
1:A:320:LYS:O	1:A:321:ILE:C	2.54	0.51
1:B:189:LEU:HD23	1:B:354:CYS:SG	2.51	0.51
1:B:212:GLN:OE1	1:B:261:LEU:HD13	2.09	0.51
1:A:236:SER:O	1:A:284:ALA:HA	2.11	0.51
1:A:165:CYS:HA	1:A:231:ALA:O	2.11	0.51
1:B:353:LEU:O	1:B:357:LEU:HB2	2.11	0.51
1:A:242:VAL:HG12	1:A:257:PRO:CA	2.41	0.50
1:A:328:LEU:HD21	1:A:367:MET:CE	2.42	0.50
1:A:360:HIS:CB	1:A:364:LEU:HD22	2.41	0.50
1:B:328:LEU:C	1:B:328:LEU:HD13	2.37	0.50
1:A:386:ILE:O	1:A:386:ILE:HG23	2.12	0.49
1:A:328:LEU:HD13	1:A:329:PHE:N	2.28	0.49
1:B:176:MET:HE3	1:B:237:HIS:HB3	1.94	0.49
1:A:364:LEU:HD21	1:A:372:ARG:CZ	2.42	0.49
1:A:166:ILE:HD11	1:A:218:ALA:HB2	1.95	0.48
1:A:333:THR:O	1:A:333:THR:HG22	2.14	0.48
1:A:163:GLY:HA3	1:A:229:CYS:O	2.13	0.48
1:A:244:TYR:CE1	1:A:255:VAL:HG13	2.48	0.48
1:B:366:ILE:HG23	1:B:367:MET:N	2.29	0.48
1:A:366:ILE:HG23	1:A:367:MET:N	2.28	0.48
1:B:171:LYS:HB2	1:B:182:THR:CG2	2.43	0.48
1:B:168:ILE:HD12	1:B:234:LEU:CD2	2.44	0.47
1:A:171:LYS:O	1:A:171:LYS:HG2	2.14	0.47
1:A:274:LEU:C	1:A:276:LYS:H	2.22	0.47
1:B:328:LEU:HD21	1:B:367:MET:CE	2.45	0.47
1:A:270:CYS:SG	1:A:273:LEU:HD12	2.55	0.47
1:B:322:PRO:HD2	1:B:329:PHE:HZ	1.78	0.47
1:A:175:LYS:C	1:A:175(B):THR:N	2.72	0.47
1:B:242:VAL:HG11	1:B:255:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PRO:HG2	1:A:260:ASP:CG	2.40	0.46
1:B:162:LYS:HG3	1:B:226:ASN:HD22	1.81	0.46
1:B:258:ILE:HD13	1:B:259:LYS:N	2.30	0.46
1:B:267:GLY:C	1:B:269:ARG:H	2.22	0.46
1:B:273:LEU:HA	1:B:276:LYS:HD2	1.98	0.46
1:A:236:SER:HB3	1:A:243:ILE:CD1	2.38	0.46
1:B:217:LYS:O	1:B:220:GLU:HB2	2.16	0.46
1:B:173:PHE:N	1:B:173:PHE:CD1	2.83	0.45
1:B:258:ILE:HA	1:B:261:LEU:HD23	1.98	0.45
1:B:355:SER:OG	1:B:376:ARG:NH2	2.48	0.45
1:A:239:GLU:HB2	1:A:242:VAL:HG23	1.97	0.45
1:B:224:HIS:H	1:B:272:THR:HB	1.81	0.45
1:B:183:ASP:HB2	2:B:1404:SO4:S	2.57	0.45
1:B:258:ILE:HD13	1:B:258:ILE:N	2.31	0.45
1:A:375:ASP:O	1:A:379:ARG:HG2	2.17	0.45
1:B:176:MET:HE3	1:B:237:HIS:CG	2.52	0.44
1:B:320:LYS:C	1:B:321:ILE:HD12	2.42	0.44
1:B:215:LEU:CD2	1:B:261:LEU:HD12	2.48	0.44
1:B:379:ARG:C	1:B:380:PHE:H	2.25	0.44
1:A:371:THR:O	1:A:374:ASN:HB2	2.18	0.44
1:B:242:VAL:CG1	1:B:243:ILE:N	2.80	0.44
1:A:328:LEU:HB2	1:A:394:LEU:HD13	2.00	0.43
1:B:151:TYR:C	1:B:396:LYS:HG3	2.42	0.43
1:B:262:THR:HG21	1:B:329:PHE:HE1	1.83	0.43
1:A:239:GLU:HB2	1:A:242:VAL:CG2	2.48	0.43
1:A:161:GLU:HB3	1:A:226:ASN:HB3	2.00	0.43
1:A:210:LYS:O	1:A:214:LEU:HG	2.19	0.43
1:A:328:LEU:HD13	1:A:328:LEU:C	2.43	0.43
1:B:320:LYS:HG3	1:B:321:ILE:CD1	2.46	0.43
1:B:215:LEU:HA	1:B:215:LEU:HD12	1.72	0.43
1:B:237:HIS:HB2	1:B:244:TYR:HB2	2.01	0.43
1:B:357:LEU:HD13	1:B:369:ILE:HG21	2.00	0.43
1:B:328:LEU:HB2	1:B:394:LEU:CD1	2.49	0.42
1:A:215:LEU:HD13	1:A:215:LEU:HA	1.90	0.42
1:B:227:ALA:O	1:B:276:LYS:NZ	2.43	0.42
1:B:153:TYR:CE2	1:B:277:PRO:HG3	2.54	0.42
1:B:204:ASN:O	1:B:205:ASP:C	2.62	0.42
1:B:149:PRO:C	1:B:151:TYR:H	2.27	0.42
1:B:259:LYS:O	1:B:263:ALA:HB2	2.19	0.42
1:A:155:MET:HG3	1:A:399:TYR:O	2.20	0.41
1:A:360:HIS:CG	1:A:364:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:HIS:HA	1:A:363:ASP:OD1	2.20	0.41
1:A:356:ILE:HG22	1:A:369:ILE:HG23	2.02	0.41
1:A:361:GLY:O	1:A:400:PHE:HB2	2.21	0.41
1:B:266:ARG:O	1:B:267:GLY:C	2.62	0.41
1:A:236:SER:OG	1:A:237:HIS:N	2.53	0.41
1:B:190:PHE:CD1	1:B:200:VAL:HG21	2.42	0.41
1:A:365:GLU:OE1	1:A:367:MET:HB2	2.20	0.41
1:A:168:ILE:CG2	1:A:211:MET:HE3	2.35	0.41
1:A:213:ASP:O	1:A:217:LYS:HG2	2.21	0.41
1:A:366:ILE:CG2	1:A:367:MET:N	2.84	0.41
1:A:173:PHE:CD1	1:A:173:PHE:N	2.88	0.41
1:A:193:PHE:O	1:A:198:PHE:HB2	2.21	0.41
1:B:196:LEU:HD23	1:B:198:PHE:CE2	2.55	0.41
1:B:192:CYS:SG	1:B:357:LEU:HD23	2.61	0.40
1:B:242:VAL:HG12	1:B:255:VAL:HB	1.95	0.40
1:A:360:HIS:HD1	1:A:364:LEU:HD13	1.85	0.40
1:B:241:ASN:OD1	1:B:320:LYS:HD2	2.21	0.40
1:B:285:ALA:HB2	1:B:334:VAL:O	2.22	0.40
1:A:266:ARG:O	1:A:269:ARG:HG3	2.21	0.40
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.85	0.40
1:B:365:GLU:CD	1:B:366:ILE:HG22	2.45	0.40
1:B:236:SER:O	1:B:284:ALA:HA	2.21	0.40
1:B:360:HIS:HA	1:B:363:ASP:OD1	2.22	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	263/265 (99%)	210 (80%)	46 (18%)	7 (3%)	4	16
1	B	261/265 (98%)	222 (85%)	29 (11%)	10 (4%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	524/530 (99%)	432 (82%)	75 (14%)	17 (3%)	3	13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	B	323	VAL
1	B	381	GLU
1	A	359	GLU
1	B	268	ASP
1	A	381(E)	ASP
1	B	335	PRO
1	A	264	HIS
1	B	317	PRO
1	B	381(G)	HIS
1	A	381(G)	HIS
1	B	141	ILE
1	B	145	ARG
1	B	341	ARG
1	A	336	GLY
1	B	293	GLY
1	A	335	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	A	233/233 (100%)	223 (96%)	10 (4%)	26	60
1	B	232/233 (100%)	216 (93%)	16 (7%)	14	41
All	All	465/466 (100%)	439 (94%)	26 (6%)	19	50

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

Mol	Chain	Res	Type
1	A	200	VAL

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Mol	Chain	Res	Type
1	A	215	LEU
1	A	220	GLU
1	A	234	LEU
1	A	272	THR
1	A	274	LEU
1	A	316	ASN
1	A	376	ARG
1	A	384	LYS
1	A	394	LEU
1	B	164	LYS
1	B	187	GLU
1	B	190	PHE
1	B	200	VAL
1	B	215	LEU
1	B	258	ILE
1	B	272	THR
1	B	274	LEU
1	B	290	LEU
1	B	320	LYS
1	B	324	GLU
1	B	362	LYS
1	B	376	ARG
1	B	382	GLU
1	B	385	GLN
1	B	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	156	ASN
1	A	169	ASN
1	A	172	ASN
1	A	204	ASN
1	A	212	GLN
1	B	283	GLN
1	B	316	ASN
1	B	379(A)	HIS
1	B	385	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](#)

5 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	$\# Z > 2$
2	SO4	B	1403	-	4,4,4	0.39	0	6,6,6	0.12	0
2	SO4	B	1405	-	4,4,4	0.42	0	6,6,6	0.10	0
2	SO4	A	1403	-	4,4,4	0.44	0	6,6,6	0.09	0
2	SO4	B	1404	-	4,4,4	0.45	0	6,6,6	0.10	0
2	SO4	B	1406	-	4,4,4	0.43	0	6,6,6	0.06	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1404	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

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.