



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:34 AM GMT

PDB ID : 1KLM
Title : HIV-1 REVERSE TRANSCRIPTASE COMPLEXED WITH BHAP U-90152
Authors : Ren, J.; Esnouf, R.M.; Stammers, D.K.; Stuart, D.I.
Deposited on : 1997-03-17
Resolution : 2.65 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

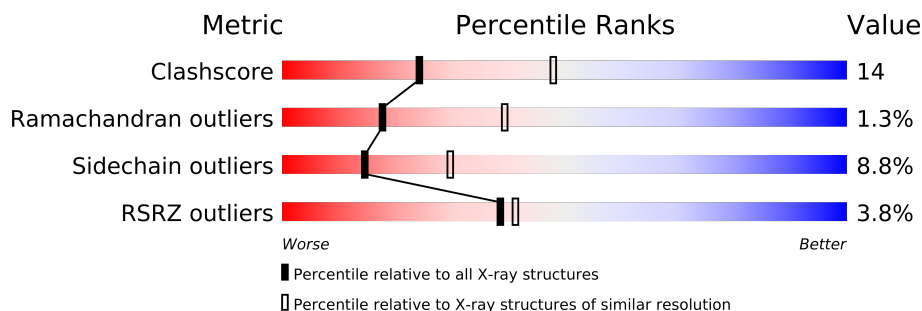
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7865 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4403	2848	733	814	8			

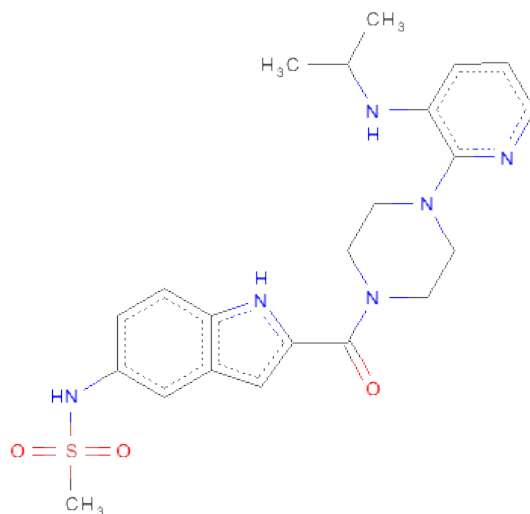
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3358	2183	558	610	7			

- Molecule 3 is (1-(5-METHANSULPHONAMIDO-1H-INDOL-2-YL-CARBONYL)4-[METHYLAMINO)PYRIDINYL]PIPERAZINE (three-letter code: SPP) (formula: C₂₂H₂₈N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	22	6	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	32	Total	O	0	0
			32	32		

GLU
THR
PHE

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.80Å 109.40Å 72.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 19.84 – 2.65	Depositor EDS
% Data completeness (in resolution range)	86.8 (20.00-2.65) 87.3 (19.84-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.67Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.237 , 0.313 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 27792 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7865	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.34	0/4511	0.61	1/6132 (0.0%)
2	B	0.34	0/3452	0.61	0/4687
All	All	0.34	0/7963	0.61	1/10819 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	N-CA-C	5.51	125.88	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4403	0	4444	134	0
2	B	3358	0	3384	85	0
3	A	32	0	28	10	0
4	A	40	0	0	0	0
4	B	32	0	0	0	0
All	All	7865	0	7856	221	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (221) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:216:THR:HB	1:A:217:PRO:HD2	1.27	1.16
1:A:225:PRO:HB2	1:A:226:PRO:HD2	1.59	0.84
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.68	0.76
1:A:358:ARG:HD2	1:A:358:ARG:O	1.86	0.76
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.68	0.75
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.87	0.74
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.67	0.74
2:B:213:GLY:C	2:B:214:LEU:HD23	2.09	0.73
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.24	0.72
2:B:84:THR:HB	2:B:154:LYS:HE2	1.71	0.72
1:A:216:THR:CB	1:A:217:PRO:HD2	2.13	0.71
1:A:2:ILE:HG22	1:A:3:SER:H	1.55	0.70
1:A:216:THR:HB	1:A:217:PRO:CD	2.16	0.70
1:A:33:ALA:O	1:A:36:GLU:HG2	1.91	0.70
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.75	0.68
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.76	0.68
3:A:999:SPP:C15	3:A:999:SPP:H112	2.23	0.67
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.78	0.66
1:A:64:LYS:H	1:A:64:LYS:HD2	1.61	0.66
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.78	0.65
1:A:516:GLU:O	1:A:520:GLN:HG3	1.96	0.65
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.78	0.64
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.77	0.64
1:A:98:ALA:HB1	1:A:383:TRP:HZ2	1.63	0.64
2:B:214:LEU:N	2:B:214:LEU:HD23	2.13	0.63
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.80	0.63
1:A:238:LYS:HB2	1:A:316:GLY:O	2.00	0.61
1:A:356:ARG:HD2	1:A:356:ARG:O	1.99	0.61
2:B:287:LYS:HE2	2:B:293:ILE:HD11	1.82	0.61
1:A:9:PRO:HG2	2:B:53:GLU:HG3	1.82	0.61
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.66	0.60
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.98	0.60
2:B:270:ILE:O	2:B:272:PRO:HD3	2.00	0.60
1:A:376:THR:O	1:A:380:ILE:HG12	2.01	0.60
1:A:46:LYS:HD3	1:A:116:PHE:HB3	1.84	0.60
1:A:335:GLY:C	1:A:356:ARG:HB3	2.23	0.59
1:A:91:GLN:NE2	1:A:95:PRO:HD3	2.18	0.59
1:A:235:HIS:ND1	1:A:238:LYS:HE2	2.18	0.59
1:A:91:GLN:HE22	1:A:95:PRO:HD3	1.67	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:106:VAL:O	2:B:233:GLU:HB2	2.04	0.58
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.39	0.57
3:A:999:SPP:H15	3:A:999:SPP:H112	1.87	0.57
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.19	0.57
1:A:31:ILE:O	1:A:35:VAL:HG23	2.05	0.57
1:A:225:PRO:HB2	1:A:226:PRO:CD	2.33	0.56
1:A:94:ILE:H	1:A:94:ILE:HD13	1.71	0.56
1:A:109:LEU:HD11	1:A:206:ARG:HH21	1.70	0.56
1:A:225:PRO:CB	1:A:226:PRO:HD2	2.33	0.56
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.41	0.56
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.86	0.55
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.40	0.55
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.41	0.55
2:B:244:ILE:HG13	2:B:426:TRP:CH2	2.41	0.55
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.88	0.55
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.88	0.55
2:B:173:LYS:O	2:B:176:PRO:HD3	2.07	0.55
1:A:106:VAL:HG21	3:A:999:SPP:H121	1.88	0.54
2:B:379:SER:CB	2:B:387:PRO:HD3	2.37	0.54
1:A:33:ALA:HA	1:A:36:GLU:OE2	2.08	0.54
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.43	0.54
1:A:3:SER:OG	1:A:5:ILE:HG22	2.08	0.54
1:A:228:LEU:CD2	1:A:233:GLU:HG2	2.39	0.53
1:A:358:ARG:HH11	1:A:358:ARG:N	2.05	0.53
2:B:267:ALA:HB2	2:B:426:TRP:NE1	2.24	0.53
2:B:64:LYS:HZ2	2:B:69:THR:HA	1.74	0.53
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.89	0.53
2:B:245:VAL:HG13	2:B:431:LYS:HB2	1.91	0.52
2:B:426:TRP:O	2:B:429:LEU:HB2	2.09	0.52
2:B:163:SER:O	2:B:167:ILE:HG22	2.09	0.52
1:A:2:ILE:HD11	1:A:45:GLY:O	2.10	0.52
3:A:999:SPP:H4	3:A:999:SPP:HB2	1.90	0.52
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.90	0.52
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.43	0.52
1:A:28:GLU:HA	1:A:135:ILE:HD11	1.91	0.52
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.92	0.51
1:A:368:LEU:O	1:A:372:VAL:HG23	2.11	0.51
1:A:98:ALA:HB2	1:A:349:LEU:O	2.10	0.51
2:B:114:ALA:HB2	2:B:214:LEU:CD1	2.41	0.51
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.40	0.51
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.92	0.51
2:B:113:ASP:HB2	2:B:214:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.93	0.51
1:A:378:GLU:O	1:A:381:VAL:HG12	2.11	0.51
1:A:524:GLN:HA	1:A:524:GLN:HE21	1.76	0.50
2:B:114:ALA:HB2	2:B:214:LEU:HD11	1.92	0.50
1:A:135:ILE:O	1:A:135:ILE:HG22	2.11	0.50
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.47	0.49
1:A:116:PHE:CE1	1:A:146:TYR:HE2	2.31	0.49
2:B:65:LYS:HD3	2:B:72:ARG:HD2	1.93	0.49
1:A:182:GLN:HG2	1:A:187:LEU:CD2	2.42	0.49
1:A:167:ILE:HG23	1:A:212:TRP:CD1	2.48	0.49
2:B:308:GLU:O	2:B:311:LYS:HB2	2.13	0.48
1:A:110:ASP:H	1:A:217:PRO:HD3	1.77	0.48
2:B:64:LYS:NZ	2:B:69:THR:HA	2.28	0.48
2:B:365:VAL:O	2:B:369:THR:HG23	2.13	0.48
2:B:50:ILE:HG22	2:B:145:GLN:OE1	2.13	0.48
1:A:293:ILE:HD12	1:A:293:ILE:N	2.29	0.48
1:A:515:SER:OG	1:A:518:VAL:HG23	2.13	0.48
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.95	0.48
1:A:332:GLN:O	1:A:336:GLN:HB2	2.13	0.48
1:A:260:LEU:O	1:A:264:LEU:HD23	2.14	0.48
2:B:111:VAL:HA	2:B:214:LEU:HD12	1.96	0.47
1:A:238:LYS:HG2	1:A:239:TRP:N	2.29	0.47
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.96	0.47
1:A:317:VAL:HG12	1:A:318:TYR:H	1.79	0.47
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.96	0.47
1:A:380:ILE:CD1	1:A:386:THR:HG22	2.43	0.47
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.47	0.47
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.50	0.47
2:B:326:ILE:O	2:B:341:ILE:HA	2.13	0.47
1:A:371:ALA:HA	1:A:374:LYS:HE3	1.95	0.47
1:A:122:GLU:CD	1:A:122:GLU:H	2.18	0.47
2:B:332:GLN:OE1	2:B:424:LYS:HG2	2.15	0.47
1:A:116:PHE:HE1	1:A:146:TYR:CE2	2.33	0.47
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.55	0.47
1:A:237:ASP:OD2	1:A:238:LYS:HD2	2.15	0.46
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.97	0.46
1:A:317:VAL:HG12	1:A:318:TYR:N	2.29	0.46
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.74	0.46
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.15	0.46
2:B:66:LYS:H	2:B:66:LYS:HD2	1.81	0.46
1:A:5:ILE:HD11	1:A:166:LYS:HD2	1.98	0.46
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:MET:HB3	1:A:185:ASP:H	1.55	0.46
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.51	0.46
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.48	0.46
2:B:421:PRO:O	2:B:425:LEU:HD22	2.16	0.46
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.43	0.46
1:A:116:PHE:HE1	1:A:146:TYR:HE2	1.62	0.46
1:A:496:VAL:HA	1:A:534:ALA:O	2.16	0.46
1:A:498:ASP:HA	1:A:536:VAL:O	2.16	0.46
1:A:66:LYS:O	1:A:68:SER:HB2	2.16	0.46
1:A:249:LYS:O	1:A:252:TRP:NE1	2.49	0.46
1:A:279:LEU:HD23	1:A:302:GLU:OE2	2.15	0.46
1:A:98:ALA:HB1	1:A:383:TRP:CZ2	2.45	0.45
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.15	0.45
2:B:31:ILE:O	2:B:35:VAL:HG23	2.16	0.45
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.31	0.45
2:B:73:LYS:HB3	2:B:73:LYS:NZ	2.32	0.45
2:B:344:GLU:HB2	2:B:347:LYS:HD2	1.99	0.45
2:B:195:ILE:HG23	2:B:196:GLY:N	2.31	0.45
1:A:475:GLN:HG3	1:A:476:LYS:N	2.32	0.45
1:A:260:LEU:HD23	1:A:279:LEU:HD11	1.99	0.45
1:A:129:ALA:HB1	1:A:143:ARG:HH12	1.82	0.45
1:A:182:GLN:HG2	1:A:187:LEU:HD21	1.98	0.45
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.52	0.45
2:B:169:GLU:HG3	2:B:173:LYS:HE3	1.99	0.45
1:A:253:THR:HA	1:A:291:GLU:O	2.17	0.45
2:B:279:LEU:HA	2:B:282:LEU:HD12	1.99	0.45
1:A:224:GLU:O	3:A:999:SPP:HE2	2.16	0.44
3:A:999:SPP:C4	3:A:999:SPP:HB2	2.48	0.44
2:B:167:ILE:HD11	2:B:209:LEU:HD12	1.99	0.44
2:B:366:LYS:O	2:B:370:GLU:HG3	2.17	0.44
1:A:518:VAL:O	1:A:522:ILE:HG13	2.18	0.44
1:A:239:TRP:HZ2	1:A:349:LEU:O	2.01	0.44
2:B:379:SER:OG	2:B:387:PRO:HD3	2.18	0.44
2:B:254:VAL:HG21	2:B:287:LYS:HG3	1.99	0.44
1:A:246:LEU:HD22	1:A:260:LEU:HD11	2.00	0.44
2:B:122:GLU:HG3	2:B:123:ASP:N	2.33	0.44
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.63	0.44
1:A:20:LYS:HG3	1:A:55:PRO:O	2.17	0.44
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.85	0.44
2:B:24:TRP:HZ3	2:B:403:THR:HG21	1.83	0.44
2:B:167:ILE:O	2:B:208:HIS:CE1	2.72	0.43
2:B:195:ILE:HG23	2:B:196:GLY:H	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:88:TRP:CZ3	2:B:57:ASN:HB2	2.53	0.43
1:A:100:LEU:HD11	3:A:999:SPP:HB1	2.00	0.43
1:A:238:LYS:HE3	1:A:240:THR:HG23	2.01	0.43
1:A:503:LEU:HA	1:A:506:ILE:HD12	2.01	0.43
1:A:454:LYS:HA	1:A:467:VAL:O	2.17	0.43
2:B:164:MET:HG2	2:B:182:GLN:NE2	2.34	0.43
2:B:303:LEU:O	2:B:307:ARG:HG3	2.19	0.43
2:B:267:ALA:HB2	2:B:426:TRP:HE1	1.82	0.43
2:B:103:LYS:HE2	2:B:179:VAL:HG23	2.00	0.43
1:A:521:ILE:O	1:A:525:LEU:HG	2.19	0.43
1:A:110:ASP:O	1:A:217:PRO:HD3	2.18	0.43
1:A:317:VAL:HG21	1:A:347:LYS:HG2	2.01	0.43
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.54	0.42
1:A:59:PRO:HG2	1:A:76:ASP:HB3	2.00	0.42
2:B:266:TRP:HZ3	2:B:426:TRP:CD2	2.38	0.42
1:A:8:VAL:O	1:A:121:ASP:HB2	2.18	0.42
1:A:91:GLN:NE2	2:B:137:ASN:O	2.52	0.42
2:B:210:LEU:C	2:B:212:TRP:H	2.23	0.42
3:A:999:SPP:H4	3:A:999:SPP:HC3	2.00	0.42
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.82	0.42
1:A:216:THR:CB	1:A:217:PRO:CD	2.88	0.42
1:A:104:LYS:HE3	1:A:104:LYS:HB2	1.87	0.42
1:A:236:PRO:HB3	3:A:999:SPP:C19	2.50	0.42
1:A:489:SER:HB2	1:A:493:VAL:HG22	2.01	0.42
2:B:107:THR:O	2:B:188:TYR:HA	2.19	0.42
1:A:475:GLN:HB2	1:A:475:GLN:HE21	1.60	0.41
1:A:244:ILE:O	1:A:244:ILE:HG23	2.21	0.41
1:A:499:SER:C	1:A:501:TYR:H	2.23	0.41
1:A:326:ILE:O	1:A:341:ILE:HA	2.19	0.41
2:B:254:VAL:O	2:B:258:GLN:HG3	2.21	0.41
2:B:43:LYS:HA	2:B:43:LYS:HD3	1.86	0.41
1:A:452:LEU:HD13	1:A:469:LEU:O	2.19	0.41
2:B:65:LYS:HB2	2:B:66:LYS:H	1.66	0.41
2:B:66:LYS:O	2:B:67:ASP:CB	2.69	0.41
2:B:201:LYS:O	2:B:204:GLU:HB3	2.21	0.41
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.02	0.41
1:A:278:GLN:HG3	1:A:298:GLU:HB3	2.03	0.41
1:A:257:ILE:O	1:A:261:VAL:HG23	2.19	0.41
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.51	0.41
2:B:353:LYS:HB2	2:B:353:LYS:HE3	1.86	0.41
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.55	0.41
1:A:357:MET:O	1:A:359:GLY:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.56	0.41
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.01	0.41
2:B:319:TYR:CZ	2:B:321:PRO:HA	2.56	0.41
2:B:175:ASN:HB3	2:B:178:ILE:HD12	2.03	0.41
1:A:436:GLY:O	1:A:461:ARG:NH2	2.53	0.41
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.56	0.41
1:A:255:ASN:OD1	1:A:289:LEU:HB3	2.19	0.41
1:A:431:LYS:HE3	1:A:431:LYS:HA	2.03	0.40
1:A:235:HIS:HB2	1:A:238:LYS:O	2.21	0.40
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.81	0.40
1:A:100:LEU:HD21	3:A:999:SPP:HB1	2.02	0.40
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.21	0.40
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.90	0.40
2:B:37:ILE:HD11	2:B:71:TRP:O	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	535/560 (96%)	482 (90%)	44 (8%)	9 (2%)	14	30
2	B	399/440 (91%)	376 (94%)	20 (5%)	3 (1%)	27	55
All	All	934/1000 (93%)	858 (92%)	64 (7%)	12 (1%)	18	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
2	B	195	ILE
1	A	230	MET
1	A	358	ARG
2	B	70	LYS
1	A	412	PRO

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Mol	Chain	Res	Type
2	B	213	GLY
1	A	66	LYS
1	A	225	PRO
1	A	14	PRO
1	A	224	GLU
1	A	345	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	482/499 (97%)	431 (89%)	51 (11%)	10	20
2	B	369/400 (92%)	345 (94%)	24 (6%)	24	48
All	All	851/899 (95%)	776 (91%)	75 (9%)	14	30

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	20	LYS
1	A	64	LYS
1	A	65	LYS
1	A	69	THR
1	A	92	LEU
1	A	94	ILE
1	A	109	LEU
1	A	113	ASP
1	A	120	LEU
1	A	123	ASP
1	A	126	LYS
1	A	139	THR
1	A	175	ASN
1	A	182	GLN
1	A	184	MET
1	A	197	GLN
1	A	205	LEU
1	A	210	LEU

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Mol	Chain	Res	Type
1	A	215	THR
1	A	238	LYS
1	A	240	THR
1	A	242	GLN
1	A	243	PRO
1	A	250	ASP
1	A	283	LEU
1	A	332	GLN
1	A	340	GLN
1	A	347	LYS
1	A	353	LYS
1	A	356	ARG
1	A	357	MET
1	A	358	ARG
1	A	362	THR
1	A	368	LEU
1	A	373	GLN
1	A	386	THR
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	413	GLU
1	A	431	LYS
1	A	448	ARG
1	A	452	LEU
1	A	475	GLN
1	A	487	GLN
1	A	491	LEU
1	A	500	GLN
1	A	515	SER
1	A	517	LEU
1	A	523	GLU
2	B	8	VAL
2	B	24	TRP
2	B	29	GLU
2	B	40	GLU
2	B	65	LYS
2	B	66	LYS
2	B	68	SER
2	B	73	LYS
2	B	167	ILE
2	B	194	GLU

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Mol	Chain	Res	Type
2	B	201	LYS
2	B	209	LEU
2	B	214	LEU
2	B	215	THR
2	B	232	TYR
2	B	233	GLU
2	B	283	LEU
2	B	284	ARG
2	B	303	LEU
2	B	338	THR
2	B	361	HIS
2	B	362	THR
2	B	368	LEU
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	174	GLN
1	A	182	GLN
1	A	221	HIS
1	A	255	ASN
1	A	336	GLN
1	A	475	GLN
1	A	500	GLN
1	A	520	GLN
1	A	524	GLN
2	B	57	ASN
2	B	161	GLN
2	B	182	GLN
2	B	235	HIS
2	B	330	GLN
2	B	332	GLN
2	B	334	GLN
2	B	340	GLN
2	B	394	GLN
2	B	428	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	CSD	A	280	1	7,7,8	6.95	2 (28%)	6,8,10	4.35	4 (66%)

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
1	CSD	A	280	1	-	1/3/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	O-C	18.11	1.23	1.11
1	A	280	CSD	CA-C	2.45	1.52	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	CA-CB-SG	7.91	122.11	110.82
1	A	280	CSD	OD2-SG-OD1	4.61	117.04	109.39
1	A	280	CSD	C-CA-N	-4.18	109.66	113.83
1	A	280	CSD	OD1-SG-CB	3.00	113.20	105.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	SPP	A	999	-	35,35,35	0.86	1 (2%)	51,51,51	0.94	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
3	SPP	A	999	-	-	0/19/31/31	0/2/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	SPP	C2-N7	2.25	1.42	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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, 95th 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	538/560 (96%)	0.00	24 (4%) 32 34	9, 44, 97, 144	0
2	B	405/440 (92%)	-0.19	12 (2%) 48 51	8, 39, 87, 112	0
All	All	943/1000 (94%)	-0.08	36 (3%) 38 41	8, 42, 92, 144	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	LYS	7.6
1	A	67	ASP	7.1
1	A	221	HIS	6.8
1	A	218	ASP	5.5
1	A	91	GLN	5.1
2	B	241	VAL	5.0
2	B	213	GLY	5.0
2	B	88	TRP	4.8
1	A	52	PRO	4.6
2	B	240	THR	4.6
1	A	137	ASN	4.3
1	A	220	LYS	4.1
2	B	67	ASP	4.0
1	A	223	LYS	3.9
2	B	232	TYR	3.9
1	A	219	LYS	3.8
1	A	356	ARG	3.4
2	B	214	LEU	3.3
1	A	69	THR	3.2
1	A	136	ASN	3.1
1	A	24	TRP	3.1
2	B	433	PRO	3.1
1	A	53	GLU	3.0
1	A	224	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	174	GLN	2.5
2	B	69	THR	2.4
1	A	22	LYS	2.4
1	A	70	LYS	2.4
1	A	358	ARG	2.3
1	A	135	ILE	2.3
2	B	6	GLU	2.3
1	A	112	GLY	2.2
1	A	68	SER	2.2
2	B	66	LYS	2.2
1	A	539	HIS	2.2
1	A	446	ALA	2.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.12	-0.77	27,31,38,41	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SPP	A	999	32/32	0.23	0.69	33,56,124,127	0

6.5 Other polymers ⓘ

There are no such residues in this entry.