



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:57 PM UTC

PDB ID : 3ALP / pdb_00003alp
Title : Cell adhesion protein
Authors : Narita, H.; Nakagawa, A.; Suzuki, M.
Deposited on : 2010-08-05
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

<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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

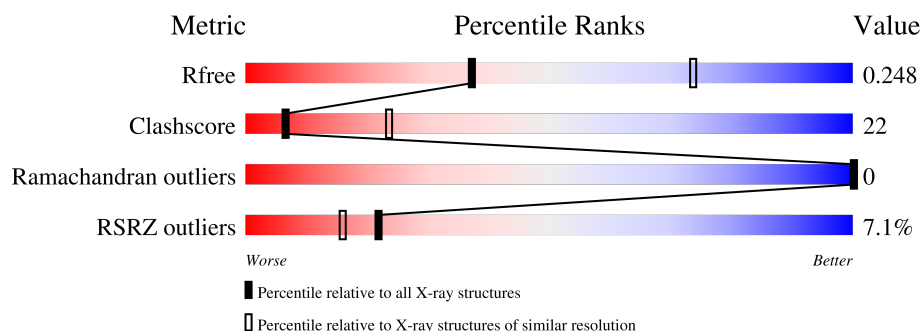
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	331	 10% 63% 26% • 9%
1	B	331	 3% 71% 20% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4727 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 Poliovirus receptor-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2299	1442	399	447	11			
1	B	304	Total	C	N	O	S	0	1	0
			2357	1479	409	458	11			

There are 50 discrepancies between the modelled and reference sequences:

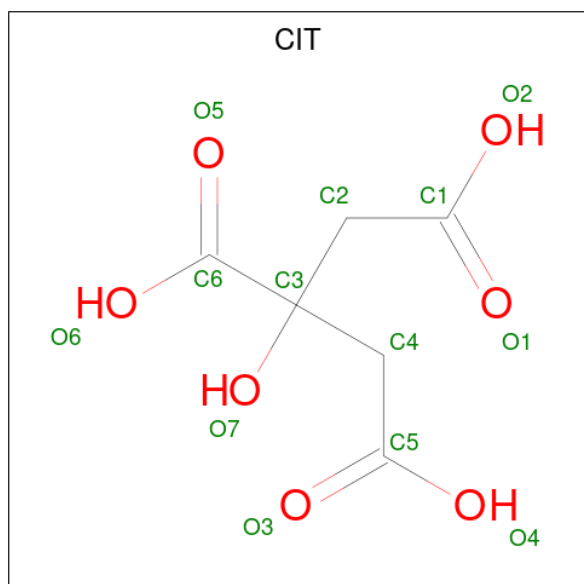
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP Q15223
A	17	ALA	-	expression tag	UNP Q15223
A	18	SER	-	expression tag	UNP Q15223
A	19	MET	-	expression tag	UNP Q15223
A	20	THR	-	expression tag	UNP Q15223
A	21	GLY	-	expression tag	UNP Q15223
A	22	GLY	-	expression tag	UNP Q15223
A	23	GLN	-	expression tag	UNP Q15223
A	24	GLN	-	expression tag	UNP Q15223
A	25	MET	-	expression tag	UNP Q15223
A	26	GLY	-	expression tag	UNP Q15223
A	27	ARG	-	expression tag	UNP Q15223
A	28	ASP	-	expression tag	UNP Q15223
A	29	PRO	-	expression tag	UNP Q15223
A	336	ALA	-	expression tag	UNP Q15223
A	337	ALA	-	expression tag	UNP Q15223
A	338	ALA	-	expression tag	UNP Q15223
A	339	LEU	-	expression tag	UNP Q15223
A	340	GLU	-	expression tag	UNP Q15223
A	341	HIS	-	expression tag	UNP Q15223
A	342	HIS	-	expression tag	UNP Q15223
A	343	HIS	-	expression tag	UNP Q15223
A	344	HIS	-	expression tag	UNP Q15223
A	345	HIS	-	expression tag	UNP Q15223
A	346	HIS	-	expression tag	UNP Q15223

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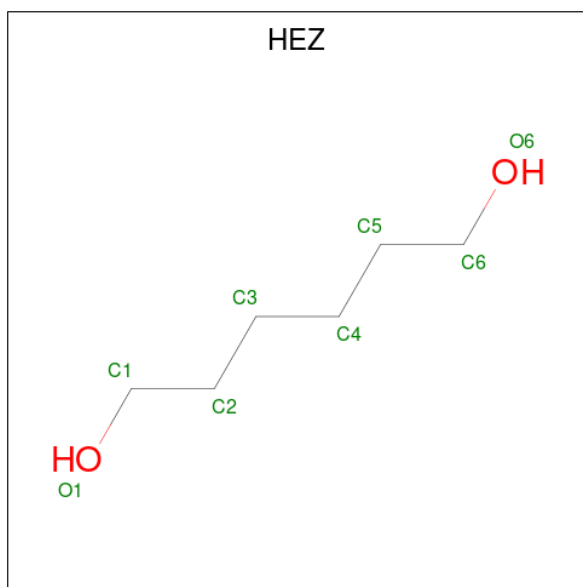
Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	expression tag	UNP Q15223
B	17	ALA	-	expression tag	UNP Q15223
B	18	SER	-	expression tag	UNP Q15223
B	19	MET	-	expression tag	UNP Q15223
B	20	THR	-	expression tag	UNP Q15223
B	21	GLY	-	expression tag	UNP Q15223
B	22	GLY	-	expression tag	UNP Q15223
B	23	GLN	-	expression tag	UNP Q15223
B	24	GLN	-	expression tag	UNP Q15223
B	25	MET	-	expression tag	UNP Q15223
B	26	GLY	-	expression tag	UNP Q15223
B	27	ARG	-	expression tag	UNP Q15223
B	28	ASP	-	expression tag	UNP Q15223
B	29	PRO	-	expression tag	UNP Q15223
B	336	ALA	-	expression tag	UNP Q15223
B	337	ALA	-	expression tag	UNP Q15223
B	338	ALA	-	expression tag	UNP Q15223
B	339	LEU	-	expression tag	UNP Q15223
B	340	GLU	-	expression tag	UNP Q15223
B	341	HIS	-	expression tag	UNP Q15223
B	342	HIS	-	expression tag	UNP Q15223
B	343	HIS	-	expression tag	UNP Q15223
B	344	HIS	-	expression tag	UNP Q15223
B	345	HIS	-	expression tag	UNP Q15223
B	346	HIS	-	expression tag	UNP Q15223

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		

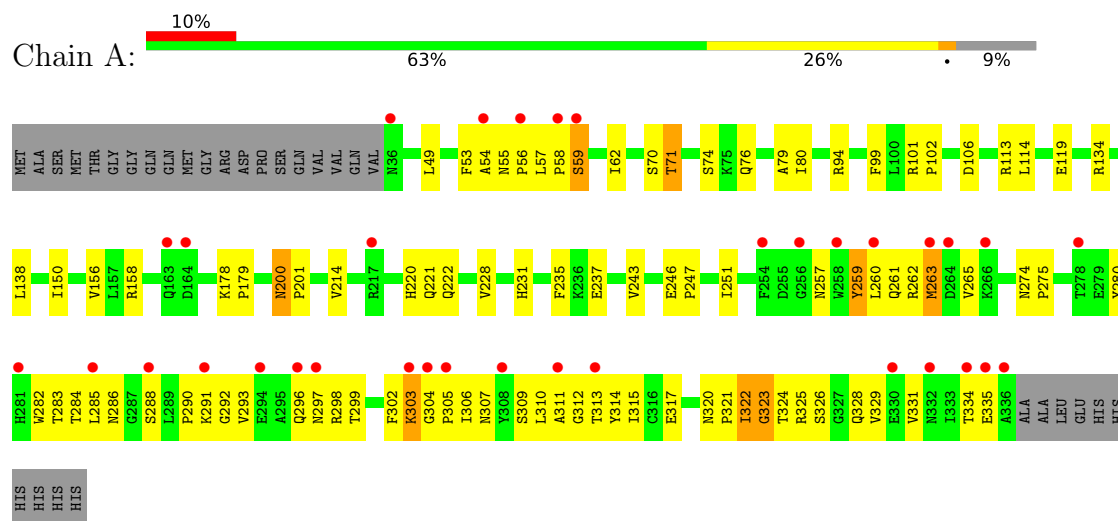
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	22	Total	O	0	0
			22	22		

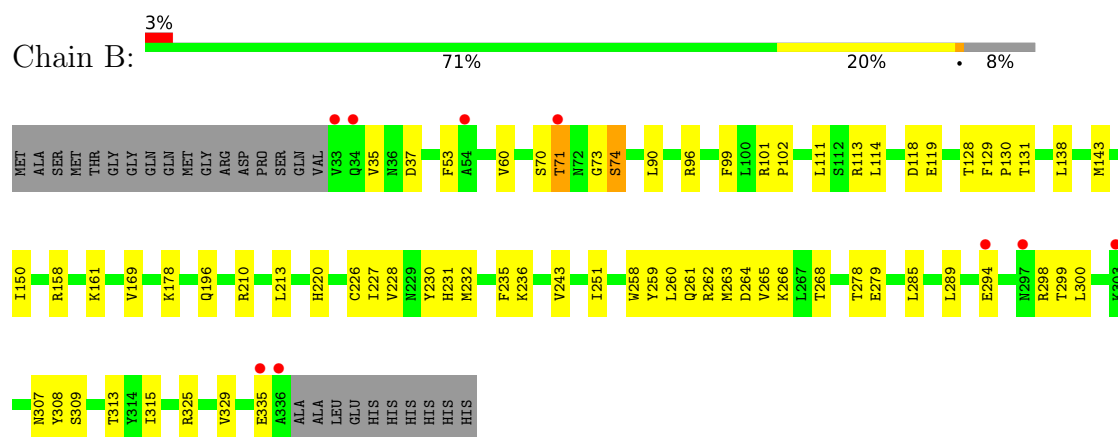
3 Residue-property plots [i](#)

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 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.

• Molecule 1: Poliovirus receptor-related protein 1



• Molecule 1: Poliovirus receptor-related protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	164.92Å 164.92Å 164.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.99 – 2.80 35.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.2 (35.99-2.80) 97.9 (35.99-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.190 , 0.226 (Not available) , 0.248	Depositor DCC
R_{free} test set	1813 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4727	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: HEZ, CIT

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	0.64	0/2350	0.93	2/3212 (0.1%)
1	B	0.57	0/2409	0.91	0/3289
All	All	0.61	0/4759	0.92	2/6501 (0.0%)

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	9
1	B	0	3
All	All	0	12

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	200	ASN	CA-C-N	5.21	125.26	119.32
1	A	200	ASN	C-N-CA	5.21	125.26	119.32

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	TYR	Peptide
1	A	263	MET	Peptide
1	A	296	GLN	Peptide
1	A	303	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	311	ALA	Peptide
1	A	322	ILE	Peptide
1	A	323	GLY	Peptide
1	A	59	SER	Peptide
1	A	71	THR	Peptide
1	B	71	THR	Peptide
1	B	73	GLY	Peptide
1	B	74	SER	Peptide

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	2299	0	2185	125	0
1	B	2357	0	2260	73	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
3	B	8	0	14	0	0
4	A	15	0	0	1	0
4	B	22	0	0	1	0
All	All	4727	0	4469	199	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 22.

All (199) 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:158:ARG:HH11	1:B:158:ARG:HG3	1.07	1.12
1:A:261:GLN:O	1:A:261:GLN:HG3	1.42	1.11
1:B:278:THR:HG22	1:B:279:GLU:HG3	1.36	1.07
1:A:56:PRO:C	1:A:57:LEU:HD23	1.82	1.03
1:A:263:MET:SD	1:A:263:MET:N	2.30	1.02
1:A:56:PRO:O	1:A:57:LEU:HD23	1.64	0.98
1:A:94:ARG:HE	1:A:94:ARG:H	0.99	0.95
1:A:113:ARG:HH11	1:A:113:ARG:HG2	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:HH11	1:A:298:ARG:CG	1.83	0.91
1:B:113:ARG:HG2	1:B:113:ARG:HH11	1.35	0.91
1:B:128:THR:OG1	1:B:131:THR:HG22	1.69	0.90
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.35	0.89
1:B:259:TYR:CE1	1:B:262:ARG:HG3	2.10	0.87
1:B:158:ARG:HG3	1:B:158:ARG:NH1	1.87	0.87
1:A:55:ASN:O	1:A:57:LEU:HD23	1.76	0.86
1:B:220:HIS:HD2	1:B:243:VAL:H	1.22	0.84
1:B:158:ARG:HH11	1:B:158:ARG:CG	1.89	0.84
1:B:259:TYR:CE1	1:B:262:ARG:HB2	2.17	0.80
1:A:55:ASN:O	1:A:57:LEU:CD2	2.30	0.79
1:A:134:ARG:HG3	1:A:134:ARG:NH1	1.96	0.78
1:A:101:ARG:O	1:A:101:ARG:CG	2.30	0.78
1:A:56:PRO:O	1:A:57:LEU:CD2	2.33	0.77
1:A:113:ARG:HH11	1:A:113:ARG:CG	1.97	0.77
1:A:322:ILE:HG22	1:A:323:GLY:CA	2.14	0.77
1:A:293:VAL:HG12	1:A:302:PHE:HD1	1.49	0.76
1:B:259:TYR:CZ	1:B:262:ARG:HG3	2.20	0.76
1:B:259:TYR:CD1	1:B:262:ARG:HB2	2.20	0.76
1:B:259:TYR:CE1	1:B:262:ARG:CG	2.69	0.75
1:A:94:ARG:HE	1:A:94:ARG:N	1.80	0.74
1:A:298:ARG:HH11	1:A:298:ARG:HG3	1.52	0.74
1:B:101:ARG:O	1:B:101:ARG:HG3	1.88	0.73
1:A:298:ARG:HG3	1:A:298:ARG:NH1	2.04	0.73
1:A:220:HIS:HD2	1:A:243:VAL:H	1.38	0.72
1:A:322:ILE:HG22	1:A:323:GLY:HA2	1.71	0.72
1:A:53:PHE:CE1	1:A:134:ARG:NH2	2.59	0.71
1:A:71:THR:CG2	1:A:71:THR:O	2.39	0.71
1:A:94:ARG:H	1:A:94:ARG:NE	1.82	0.71
1:A:246:GLU:CA	1:A:322:ILE:HG21	2.21	0.70
1:A:315:ILE:HG22	1:A:328:GLN:HG2	1.73	0.70
1:A:306:ILE:HG23	1:A:310:LEU:HD12	1.73	0.70
1:A:53:PHE:C	1:A:53:PHE:HD1	1.99	0.70
1:A:324:THR:O	1:A:325:ARG:HG2	1.92	0.70
1:A:312:GLY:H	1:A:331:VAL:HG12	1.56	0.69
1:A:101:ARG:O	1:A:101:ARG:HG3	1.91	0.69
1:A:53:PHE:HD1	1:A:54:ALA:N	1.90	0.68
1:B:259:TYR:CE1	1:B:262:ARG:CB	2.76	0.68
1:B:113:ARG:HH11	1:B:113:ARG:CG	2.05	0.68
1:A:320:ASN:OD1	1:A:320:ASN:C	2.37	0.67
1:A:293:VAL:HG12	1:A:302:PHE:CD1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:SER:HB2	1:B:74:SER:O	1.97	0.65
1:A:280:TYR:CD1	1:A:298:ARG:HB2	2.32	0.65
1:A:246:GLU:N	1:A:322:ILE:HG21	2.11	0.64
1:A:290:PRO:O	1:A:293:VAL:HG13	1.98	0.64
1:A:312:GLY:H	1:A:331:VAL:CG1	2.11	0.64
1:A:320:ASN:OD1	1:A:321:PRO:N	2.30	0.64
1:A:220:HIS:CE1	1:A:221:GLN:HG3	2.32	0.64
1:A:261:GLN:O	1:A:261:GLN:CG	2.30	0.63
1:B:285:LEU:HD13	1:B:315:ILE:HD11	1.80	0.63
1:A:297:ASN:OD1	1:A:297:ASN:N	2.30	0.63
1:B:70:SER:HA	1:B:74:SER:O	1.99	0.63
1:A:317:GLU:HG2	1:A:326:SER:HB3	1.81	0.63
1:B:268:THR:HG22	1:B:299:THR:HB	1.81	0.63
1:B:169:VAL:HG21	1:B:213:LEU:HD22	1.81	0.62
1:B:307:ASN:HD22	1:B:309:SER:H	1.45	0.62
1:A:303:LYS:O	1:A:305:PRO:HD2	1.98	0.62
1:A:259:TYR:HB3	1:A:260:LEU:O	2.00	0.62
1:B:260:LEU:HD21	1:B:308:TYR:CE2	2.36	0.61
1:B:101:ARG:O	1:B:101:ARG:CG	2.46	0.61
1:A:70:SER:HA	1:A:74:SER:O	2.02	0.60
1:A:293:VAL:CG1	1:A:302:PHE:CD1	2.85	0.60
1:B:213:LEU:HD23	1:B:213:LEU:C	2.27	0.60
1:A:53:PHE:C	1:A:53:PHE:CD1	2.71	0.59
1:A:99:PHE:HB2	1:A:102:PRO:HG3	1.83	0.59
1:A:293:VAL:CG1	1:A:302:PHE:HD1	2.16	0.59
1:A:307:ASN:HD21	1:A:310:LEU:HG	1.67	0.59
1:B:285:LEU:CD1	1:B:315:ILE:HD11	2.33	0.59
1:A:320:ASN:O	1:A:323:GLY:N	2.30	0.59
1:A:307:ASN:ND2	1:A:310:LEU:HG	2.17	0.58
1:B:53:PHE:C	1:B:53:PHE:CD1	2.81	0.58
1:B:307:ASN:ND2	1:B:309:SER:HB3	2.18	0.58
1:A:298:ARG:HH11	1:A:298:ARG:HG2	1.64	0.58
1:A:119:GLU:OE2	1:A:178:LYS:NZ	2.32	0.57
1:B:325:ARG:HG2	1:B:325:ARG:HH11	1.69	0.57
1:A:134:ARG:HH11	1:A:134:ARG:CG	2.12	0.57
1:B:220:HIS:HD2	1:B:243:VAL:N	2.00	0.57
1:A:57:LEU:HB3	1:A:58:PRO:CD	2.35	0.57
1:A:57:LEU:HB3	1:A:58:PRO:HD2	1.87	0.57
1:A:71:THR:O	1:A:71:THR:HG22	2.04	0.56
1:A:259:TYR:CB	1:A:260:LEU:O	2.53	0.56
1:A:283:THR:HG22	1:A:284:THR:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TRP:CE2	1:B:265:VAL:HG21	2.41	0.56
1:A:309:SER:O	1:A:310:LEU:HB2	2.06	0.56
1:B:260:LEU:O	1:B:261:GLN:CB	2.54	0.56
1:B:251:ILE:HB	1:B:329:VAL:HG13	1.88	0.55
1:A:320:ASN:OD1	1:A:322:ILE:N	2.36	0.55
1:A:297:ASN:O	1:A:298:ARG:HB3	2.07	0.55
1:A:312:GLY:O	1:A:331:VAL:HG12	2.07	0.55
1:B:298:ARG:O	1:B:298:ARG:HG3	2.07	0.55
1:A:58:PRO:CD	1:A:59:SER:H	2.20	0.54
1:A:214:VAL:HG12	4:A:349:HOH:O	2.07	0.54
1:B:99:PHE:CB	1:B:102:PRO:HG3	2.37	0.54
1:A:246:GLU:CB	1:A:322:ILE:HG21	2.38	0.53
1:A:53:PHE:CD1	1:A:54:ALA:N	2.75	0.53
1:A:265:VAL:O	1:A:265:VAL:CG1	2.56	0.52
1:B:143:MET:SD	1:B:231[B]:HIS:HE1	2.32	0.52
1:A:56:PRO:C	1:A:57:LEU:CD2	2.71	0.52
1:A:222:GLN:NE2	1:A:222:GLN:HA	2.25	0.52
1:B:258:TRP:NE1	1:B:265:VAL:HG21	2.26	0.51
1:B:307:ASN:HD22	1:B:309:SER:N	2.08	0.51
1:A:113:ARG:CG	1:A:113:ARG:NH1	2.65	0.51
1:A:274:ASN:HA	1:A:275:PRO:C	2.35	0.51
1:B:70:SER:CA	1:B:74:SER:O	2.59	0.50
1:A:284:THR:HG23	1:A:286:ASN:H	1.76	0.50
1:B:71:THR:O	1:B:74:SER:OG	2.30	0.50
1:B:150:ILE:HD12	1:B:226:CYS:HB3	1.94	0.49
1:A:280:TYR:CG	1:A:298:ARG:HB2	2.46	0.49
1:B:35:VAL:HG11	1:B:138:LEU:HA	1.94	0.49
2:A:1:CIT:O4	2:A:1:CIT:H21	2.12	0.49
1:A:247:PRO:HD3	1:A:320:ASN:ND2	2.27	0.49
1:B:60:VAL:O	1:B:60:VAL:HG23	2.13	0.49
1:B:99:PHE:HB3	1:B:102:PRO:HG3	1.94	0.49
1:A:297:ASN:C	1:A:299:THR:H	2.21	0.48
1:B:220:HIS:CD2	1:B:243:VAL:H	2.14	0.48
1:B:335:GLU:HG2	1:B:335:GLU:O	2.13	0.48
1:A:251:ILE:HB	1:A:329:VAL:HG23	1.95	0.48
1:A:315:ILE:O	1:A:315:ILE:HG13	2.14	0.48
1:A:156:VAL:HG21	1:A:158:ARG:NH2	2.29	0.48
1:B:138:LEU:C	1:B:138:LEU:HD12	2.39	0.48
1:A:298:ARG:CG	1:A:298:ARG:O	2.61	0.48
1:A:291:LYS:HA	1:A:292:GLY:HA2	1.60	0.48
1:B:70:SER:CB	1:B:74:SER:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:VAL:O	1:A:331:VAL:HG13	2.15	0.47
1:A:57:LEU:HD22	1:A:57:LEU:HA	1.70	0.47
1:A:58:PRO:HD2	1:A:59:SER:H	1.78	0.47
1:A:297:ASN:O	1:A:298:ARG:CB	2.62	0.47
1:A:285:LEU:CB	1:A:313:THR:HB	2.45	0.47
1:B:259:TYR:CD1	1:B:259:TYR:C	2.93	0.47
1:A:220:HIS:NE2	1:A:274:ASN:ND2	2.62	0.46
1:A:282:TRP:HE1	1:A:298:ARG:H	1.62	0.46
1:B:35:VAL:HG12	1:B:37:ASP:H	1.81	0.46
1:A:262:ARG:O	1:A:304:GLY:O	2.34	0.46
1:B:228:VAL:HB	1:B:235:PHE:HB3	1.98	0.46
1:A:62:ILE:HD12	1:A:62:ILE:N	2.31	0.45
1:A:309:SER:O	1:A:310:LEU:CB	2.64	0.45
1:A:114:LEU:HD12	1:A:114:LEU:HA	1.82	0.45
1:A:314:TYR:O	1:A:328:GLN:HA	2.17	0.45
1:A:334:THR:HG22	1:A:335:GLU:H	1.81	0.45
1:A:80:ILE:N	1:A:80:ILE:HD12	2.32	0.45
1:A:99:PHE:CB	1:A:102:PRO:HG3	2.46	0.45
1:A:284:THR:CG2	1:A:288:SER:O	2.65	0.45
1:B:227:ILE:CD1	1:B:236:LYS:HD2	2.47	0.45
1:A:150:ILE:HG22	1:A:237:GLU:CD	2.43	0.44
1:B:265:VAL:HG22	1:B:266:LYS:N	2.31	0.44
1:A:324:THR:HG22	1:A:325:ARG:N	2.32	0.44
1:B:161:LYS:HE2	1:B:161:LYS:H	1.81	0.44
1:A:79:ALA:C	1:A:80:ILE:HD12	2.42	0.44
1:B:113:ARG:CG	1:B:113:ARG:NH1	2.72	0.44
1:B:307:ASN:HD22	1:B:307:ASN:C	2.25	0.44
1:A:101:ARG:O	1:A:101:ARG:HG2	2.16	0.44
1:A:257:ASN:OD1	1:A:259:TYR:HE2	2.01	0.44
1:A:265:VAL:CG1	1:A:302:PHE:HD2	2.31	0.44
1:A:53:PHE:CD1	1:A:134:ARG:NH2	2.86	0.43
1:A:101:ARG:HD2	1:A:106:ASP:OD2	2.17	0.43
1:B:289:LEU:HD21	1:B:300:LEU:HD11	2.00	0.43
1:A:247:PRO:HG3	1:A:320:ASN:HD22	1.82	0.43
1:A:320:ASN:CB	1:A:321:PRO:CD	2.96	0.43
1:A:200:ASN:HB3	1:A:201:PRO:HD2	2.00	0.43
1:A:265:VAL:O	1:A:265:VAL:HG13	2.18	0.43
1:B:294:GLU:HA	1:B:294:GLU:OE2	2.18	0.43
1:A:283:THR:HG22	1:A:284:THR:H	1.82	0.43
1:B:129:PHE:CG	1:B:130:PRO:HA	2.53	0.43
1:A:322:ILE:HD12	1:A:322:ILE:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:HIS:O	1:A:231:HIS:CG	2.73	0.42
1:A:246:GLU:CB	1:A:322:ILE:CG2	2.98	0.42
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.85	0.42
1:A:76:GLN:HE21	1:A:76:GLN:HB2	1.71	0.42
1:B:96:ARG:NH2	1:B:118:ASP:OD2	2.52	0.42
1:A:49:LEU:HD22	1:A:138:LEU:HD11	2.02	0.42
1:A:293:VAL:HG11	1:A:302:PHE:CE1	2.54	0.42
1:B:90:LEU:HD23	1:B:90:LEU:N	2.34	0.42
1:A:71:THR:O	1:A:71:THR:HG23	2.13	0.42
1:B:260:LEU:O	1:B:261:GLN:HB3	2.20	0.42
1:B:231[B]:HIS:O	1:B:232:MET:HB2	2.19	0.41
1:A:55:ASN:C	1:A:57:LEU:HD23	2.42	0.41
1:A:178:LYS:HA	1:A:179:PRO:C	2.45	0.41
1:A:228:VAL:HG13	1:A:235:PHE:CD1	2.56	0.41
1:B:235:PHE:CD1	1:B:235:PHE:C	2.99	0.41
1:B:263:MET:O	1:B:264:ASP:C	2.63	0.41
1:B:111:LEU:HD13	1:B:114:LEU:CD1	2.51	0.41
1:B:230:TYR:O	1:B:231[A]:HIS:C	2.63	0.41
1:B:119:GLU:OE2	1:B:178:LYS:NZ	2.52	0.41
1:B:196:GLN:OE1	1:B:210:ARG:NH2	2.53	0.41
1:B:285:LEU:HB2	1:B:313:THR:HB	2.03	0.41
1:A:314:TYR:HE2	1:A:331:VAL:HG11	1.85	0.41
1:B:231[A]:HIS:O	1:B:232:MET:HB2	2.21	0.41
1:A:222:GLN:CA	1:A:222:GLN:HE21	2.33	0.41
1:A:228:VAL:HG13	1:A:235:PHE:HD1	1.86	0.41
1:B:74:SER:HA	4:B:358:HOH:O	2.20	0.40
1:B:251:ILE:HB	1:B:329:VAL:CG1	2.50	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	A	299/331 (90%)	286 (96%)	13 (4%)	0	100	100
1	B	303/331 (92%)	293 (97%)	10 (3%)	0	100	100
All	All	602/662 (91%)	579 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

3 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	CIT	A	1	-	12,12,12	1.08	0	17,17,17	1.61	3 (17%)
2	CIT	B	2	-	12,12,12	1.05	0	17,17,17	1.45	3 (17%)
3	HEZ	B	1	-	7,7,7	0.26	0	6,6,6	0.75	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
2	CIT	A	1	-	-	9/16/16/16	-
2	CIT	B	2	-	-	4/16/16/16	-
3	HEZ	B	1	-	-	3/5/5/5	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	CIT	O6-C6-C3	3.81	120.44	113.14
2	B	2	CIT	O6-C6-C3	3.49	119.84	113.14
2	A	1	CIT	O2-C1-C2	2.77	123.14	114.35
2	B	2	CIT	O4-C5-C4	2.45	122.10	114.35
2	A	1	CIT	O2-C1-O1	-2.18	117.73	123.33
2	B	2	CIT	C3-C4-C5	-2.07	108.27	113.92

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	CIT	C1-C2-C3-O7
2	A	1	CIT	C1-C2-C3-C6
2	A	1	CIT	O7-C3-C6-O5
2	A	1	CIT	O7-C3-C6-O6
2	A	1	CIT	C4-C3-C6-O5
2	A	1	CIT	C4-C3-C6-O6
2	A	1	CIT	C1-C2-C3-C4
2	B	2	CIT	C1-C2-C3-O7
2	B	2	CIT	C1-C2-C3-C4
2	B	2	CIT	C1-C2-C3-C6
3	B	1	HEZ	C1-C2-C3-C4
3	B	1	HEZ	C4-C5-C6-O6
2	B	2	CIT	C2-C3-C4-C5
3	B	1	HEZ	C3-C4-C5-C6
2	A	1	CIT	O2-C1-C2-C3
2	A	1	CIT	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	CIT	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

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	301/331 (90%)	0.29	34 (11%) 10 7	38, 76, 168, 230	0
1	B	304/331 (91%)	-0.13	9 (2%) 52 42	29, 66, 123, 164	1 (0%)
All	All	605/662 (91%)	0.08	43 (7%) 22 16	29, 69, 153, 230	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	GLY	5.1
1	B	335	GLU	5.1
1	A	294	GLU	5.0
1	A	263	MET	4.6
1	B	71	THR	4.5
1	A	260	LEU	4.5
1	B	33	VAL	4.3
1	A	291	LYS	4.2
1	A	335	GLU	3.8
1	A	256	GLY	3.8
1	A	313	THR	3.7
1	A	164	ASP	3.6
1	A	305	PRO	3.6
1	B	336	ALA	3.6
1	A	303	LYS	3.5
1	A	254	PHE	3.4
1	A	336	ALA	3.3
1	A	264	ASP	3.2
1	A	311	ALA	3.2
1	A	308	TYR	3.2
1	B	34	GLN	3.1
1	A	330	GLU	3.0
1	A	285	LEU	2.9
1	B	297	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	281	HIS	2.9
1	A	217	ARG	2.8
1	A	258	TRP	2.6
1	B	54	ALA	2.6
1	A	266	LYS	2.6
1	A	54	ALA	2.6
1	A	288	SER	2.5
1	B	294	GLU	2.5
1	A	56	PRO	2.5
1	A	278	THR	2.5
1	A	59	SER	2.4
1	A	334	THR	2.4
1	B	303	LYS	2.3
1	A	296	GLN	2.3
1	A	297	ASN	2.1
1	A	163	GLN	2.1
1	A	36	ASN	2.1
1	A	332	ASN	2.1
1	A	58	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	B	2	13/13	0.91	0.12	88,100,128,131	0
2	CIT	A	1	13/13	0.94	0.10	91,114,124,125	0
3	HEZ	B	1	8/8	0.95	0.12	55,57,69,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.