



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:23 PM UTC

PDB ID : 1JNF / pdb_00001jnf
Title : Rabbit serum transferrin at 2.6 Å resolution.
Authors : Hall, D.R.; Hadden, J.M.; Leonard, G.A.; Bailey, S.; Neu, M.; Winn, M.;
Lindley, P.F.
Deposited on : 2001-07-24
Resolution : 2.60 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

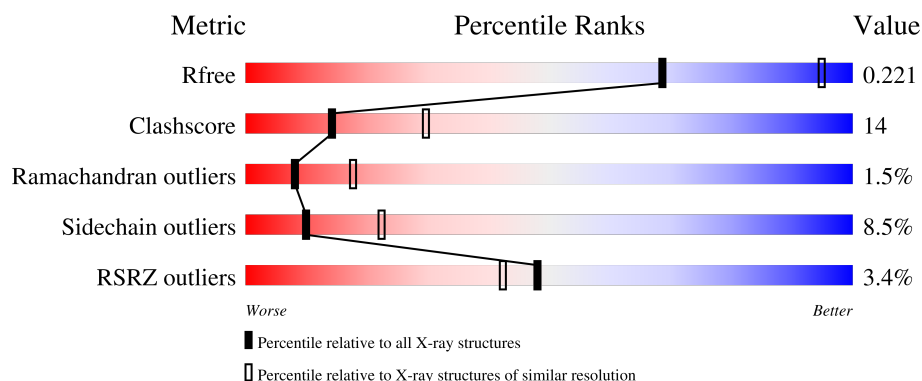
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	676	3% 65% 29% 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5433 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.

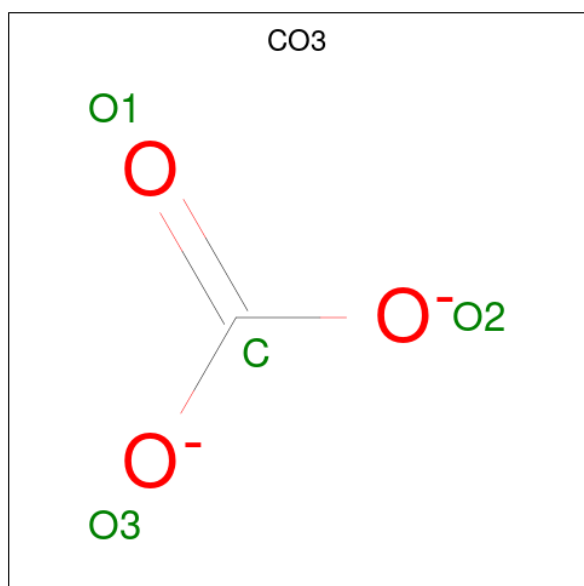
- Molecule 1 is a protein called serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	674	5216	3281	905	986	44	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	LEU	TYR	conflict	UNP P19134
A	348	GLY	SER	conflict	UNP P19134
A	605	PHE	TYR	conflict	UNP P19134

- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	1	3	0	0
2	A	1	4	1	3	0	0

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Fe 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total 206	O 206	0	0

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 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: serotransferrin



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.19Å 127.19Å 144.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.60) 97.5 (30.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.185 , 0.223 0.186 , 0.221	Depositor DCC
R_{free} test set	1808 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5433	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: CO3, FE, CL

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	1.26	16/5332 (0.3%)	1.27	24/7207 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	578	LYS	C-O	-8.28	1.14	1.23
1	A	132	ILE	CA-CB	-6.41	1.46	1.54
1	A	536	LEU	C-O	-6.39	1.16	1.24
1	A	134	LEU	C-O	-6.15	1.16	1.24
1	A	535	VAL	C-O	-5.88	1.17	1.24
1	A	383	ASN	N-CA	-5.79	1.39	1.46
1	A	431	VAL	CA-CB	-5.63	1.46	1.54
1	A	530	VAL	CA-C	-5.55	1.45	1.52
1	A	113	GLN	C-O	-5.42	1.17	1.23
1	A	130	ILE	CA-CB	-5.18	1.47	1.54
1	A	16	ALA	CA-CB	-5.16	1.45	1.53
1	A	484	ALA	CA-CB	-5.16	1.46	1.53
1	A	669	GLU	C-O	-5.12	1.18	1.24
1	A	460	ASN	C-O	-5.10	1.18	1.24
1	A	460	ASN	CA-C	-5.08	1.46	1.52
1	A	17	SER	CA-C	-5.02	1.46	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASP	N-CA-C	7.78	119.40	111.07
1	A	479	PHE	N-CA-C	-7.28	99.74	110.52
1	A	249	HIS	N-CA-C	-7.00	99.92	110.28
1	A	403	GLY	N-CA-C	5.92	123.24	115.36
1	A	664	THR	N-CA-C	-5.78	103.68	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ILE	N-CA-C	-5.71	105.16	110.53
1	A	502	VAL	N-CA-C	5.51	115.51	108.12
1	A	73	THR	N-CA-C	-5.48	102.52	110.08
1	A	433	LYS	N-CA-C	-5.45	105.42	111.36
1	A	106	ASN	N-CA-C	5.36	122.23	110.80
1	A	391	LEU	N-CA-C	5.35	117.53	109.23
1	A	37	ILE	CA-C-N	-5.34	116.14	123.14
1	A	37	ILE	C-N-CA	-5.34	116.14	123.14
1	A	368	CYS	N-CA-C	5.34	117.22	108.52
1	A	273	HIS	N-CA-C	5.33	119.86	112.45
1	A	401	GLN	N-CA-C	-5.27	105.71	111.82
1	A	251	VAL	CB-CA-C	-5.23	104.97	111.08
1	A	306	PRO	CA-C-N	5.20	124.99	119.28
1	A	306	PRO	C-N-CA	5.20	124.99	119.28
1	A	105	SER	N-CA-C	-5.17	106.97	113.28
1	A	482	GLY	N-CA-C	5.12	118.95	110.55
1	A	318	GLU	N-CA-CB	5.06	117.32	109.98
1	A	636	VAL	N-CA-C	5.05	115.86	108.53
1	A	281	ASP	N-CA-C	-5.00	106.02	111.82

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	5216	0	5060	146	0
2	A	8	0	0	0	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	206	0	0	6	0
All	All	5433	0	5060	146	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 14.

All (146) 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:623:THR:HG22	1:A:624:LYS:H	1.05	1.09
1:A:623:THR:HG22	1:A:624:LYS:N	1.83	0.92
1:A:328:GLU:HB3	1:A:330:ILE:HG12	1.52	0.92
1:A:379:ALA:HA	1:A:382:MET:CE	2.09	0.83
1:A:497:CYS:HB3	1:A:509:GLU:OE1	1.80	0.81
1:A:382:MET:HE1	1:A:667:LEU:HD11	1.62	0.80
1:A:33:ASP:O	1:A:34:GLY:O	2.00	0.79
1:A:7:ARG:HH11	1:A:7:ARG:HG3	1.49	0.77
1:A:254:ARG:NH1	1:A:257:ASP:O	2.17	0.76
1:A:33:ASP:O	1:A:34:GLY:C	2.29	0.74
1:A:357:GLU:HG2	1:A:616:PHE:CE1	2.24	0.72
1:A:343:LYS:HD3	1:A:367:GLU:HB3	1.71	0.71
1:A:480:ARG:HA	1:A:480:ARG:NH1	2.05	0.71
1:A:418:LYS:O	1:A:639:ARG:NH2	2.23	0.71
1:A:407:VAL:HG13	1:A:408:LEU:N	2.03	0.71
1:A:643:THR:HB	1:A:646:LYS:HD2	1.71	0.71
1:A:379:ALA:HA	1:A:382:MET:HE2	1.72	0.71
1:A:453:VAL:HG13	1:A:485:PRO:O	1.91	0.69
1:A:304:LYS:HD3	1:A:305:VAL:N	2.09	0.67
1:A:347:LEU:O	1:A:348:GLY:O	2.13	0.66
1:A:375:GLU:OE2	1:A:665:SER:OG	2.06	0.66
1:A:316:GLY:O	1:A:320:VAL:HG23	1.97	0.65
1:A:379:ALA:HA	1:A:382:MET:HE3	1.79	0.65
1:A:499:GLY:HA3	1:A:509:GLU:HA	1.79	0.64
1:A:407:VAL:HG13	1:A:408:LEU:H	1.60	0.63
1:A:476:ASP:HB2	1:A:492:SER:OG	1.99	0.62
1:A:33:ASP:C	1:A:34:GLY:O	2.41	0.62
1:A:592:ALA:O	1:A:593:CYS:C	2.43	0.61
1:A:7:ARG:NH1	1:A:58:ASP:OD1	2.33	0.61
1:A:357:GLU:HG2	1:A:616:PHE:CD1	2.37	0.60
1:A:643:THR:HG22	1:A:646:LYS:H	1.67	0.59
1:A:657:SER:HA	1:A:660:ARG:HG2	1.85	0.59
1:A:461:ILE:HB	1:A:462:PRO:HD3	1.84	0.59
1:A:588:LYS:O	1:A:589:ASP:C	2.44	0.58
1:A:444:GLU:HG2	1:A:478:PHE:CE2	2.37	0.58
1:A:623:THR:CG2	1:A:624:LYS:N	2.55	0.58
1:A:206:LYS:NZ	1:A:296:LYS:NZ	2.51	0.58
1:A:669:GLU:OE2	5:A:947:HOH:O	2.18	0.57
1:A:424:GLY:HA2	1:A:581:ASN:OD1	2.05	0.56
1:A:333:ASP:O	1:A:335:LEU:N	2.38	0.56
1:A:185:TYR:C	1:A:190:GLY:HA3	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:CG1	1:A:408:LEU:N	2.68	0.55
1:A:607:ASN:OD1	1:A:608:THR:N	2.39	0.55
1:A:499:GLY:O	1:A:500:PRO:C	2.48	0.55
1:A:407:VAL:CG1	1:A:408:LEU:H	2.18	0.55
1:A:615:LYS:HG2	1:A:616:PHE:N	2.20	0.55
1:A:7:ARG:NH1	1:A:58:ASP:OD2	2.40	0.55
1:A:249:HIS:CE1	1:A:296:LYS:HD2	2.41	0.55
1:A:54:ALA:O	1:A:55:HIS:HB2	2.07	0.55
1:A:377:CYS:HB3	1:A:389:MET:SD	2.47	0.54
1:A:463:MET:HE3	1:A:475:PHE:HB3	1.89	0.54
1:A:481:GLN:HE21	1:A:495:GLU:HB3	1.73	0.54
1:A:362:SER:O	1:A:365:LEU:HD12	2.08	0.54
1:A:116:LYS:NZ	5:A:977:HOH:O	2.42	0.53
1:A:395:TYR:OH	5:A:956:HOH:O	2.17	0.53
1:A:452:ALA:HB3	1:A:455:ARG:HD3	1.91	0.53
1:A:359:SER:O	1:A:360:VAL:C	2.50	0.53
1:A:18:LYS:HD3	1:A:294:LEU:HD12	1.91	0.53
1:A:467:TYR:C	1:A:469:ARG:H	2.17	0.53
1:A:117:SER:OG	1:A:157:SER:OG	2.22	0.53
1:A:19:CYS:O	1:A:22:PHE:HB3	2.09	0.52
1:A:621:SER:HB3	1:A:630:ASP:OD1	2.09	0.52
1:A:382:MET:SD	1:A:402:CYS:HB3	2.50	0.51
1:A:137:CYS:O	1:A:143:ARG:NH2	2.43	0.51
1:A:498:VAL:HG23	1:A:499:GLY:N	2.24	0.51
1:A:32:GLU:H	1:A:32:GLU:CD	2.19	0.51
1:A:139:LEU:HB3	1:A:140:PRO:HD2	1.94	0.50
1:A:58:ASP:OD1	1:A:254:ARG:NH2	2.45	0.50
1:A:7:ARG:NH2	1:A:55:HIS:O	2.25	0.50
1:A:158:CYS:SG	1:A:160:PRO:HD3	2.52	0.50
1:A:381:ILE:HA	1:A:386:ALA:O	2.10	0.50
1:A:499:GLY:HA3	1:A:510:GLY:H	1.77	0.50
1:A:548:ALA:HA	1:A:551:LEU:CD1	2.42	0.50
1:A:265:GLU:O	1:A:269:GLN:HG2	2.11	0.50
1:A:541:GLY:HA2	1:A:549:LYS:HD2	1.94	0.50
1:A:320:VAL:O	1:A:324:ARG:HB2	2.12	0.50
1:A:308:ARG:HB2	1:A:666:ARG:HB3	1.94	0.49
1:A:498:VAL:O	1:A:499:GLY:C	2.56	0.48
1:A:595:LYS:O	1:A:598:LEU:N	2.46	0.48
1:A:392:ASP:HA	1:A:582:HIS:CD2	2.49	0.48
1:A:7:ARG:NH1	1:A:58:ASP:CG	2.71	0.48
1:A:206:LYS:HZ2	1:A:296:LYS:NZ	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LYS:HD3	1:A:304:LYS:C	2.36	0.47
1:A:433:LYS:HD2	1:A:554:GLU:O	2.14	0.47
1:A:31:PRO:O	1:A:33:ASP:N	2.47	0.47
1:A:570:GLU:O	1:A:571:ALA:C	2.58	0.47
1:A:392:ASP:HB2	1:A:582:HIS:CE1	2.49	0.47
1:A:499:GLY:CA	1:A:510:GLY:H	2.28	0.47
1:A:498:VAL:O	1:A:499:GLY:O	2.32	0.47
1:A:548:ALA:HA	1:A:551:LEU:HG	1.97	0.47
1:A:73:THR:CG2	1:A:74:PRO:HA	2.45	0.47
1:A:483:CYS:HB2	1:A:496:LEU:HB2	1.97	0.47
1:A:258:GLY:HA2	5:A:924:HOH:O	2.15	0.47
1:A:324:ARG:O	1:A:328:GLU:HB2	2.14	0.47
1:A:308:ARG:O	1:A:308:ARG:HD2	2.14	0.46
1:A:130:ILE:HB	1:A:131:PRO:CD	2.45	0.46
1:A:310:ASP:OD1	1:A:313:LEU:HB2	2.15	0.46
1:A:347:LEU:O	1:A:351:GLU:HB2	2.16	0.46
1:A:272:GLU:OE1	1:A:272:GLU:HA	2.15	0.46
1:A:521:LEU:HB2	1:A:528:ALA:HB2	1.98	0.46
1:A:81:VAL:CG1	1:A:302:PHE:HB3	2.46	0.46
1:A:514:TYR:HE2	1:A:629:ARG:HD2	1.81	0.45
1:A:445:GLY:O	1:A:480:ARG:HB2	2.17	0.45
1:A:332:PRO:C	1:A:333:ASP:O	2.59	0.44
1:A:296:LYS:HG3	5:A:831:HOH:O	2.17	0.44
1:A:73:THR:HG23	1:A:74:PRO:HA	2.00	0.44
1:A:488:GLN:O	1:A:490:ASN:N	2.50	0.44
1:A:605:PHE:CE1	1:A:616:PHE:HB3	2.53	0.43
1:A:206:LYS:NZ	1:A:296:LYS:HZ1	2.16	0.43
1:A:333:ASP:OD1	1:A:333:ASP:N	2.50	0.43
1:A:467:TYR:C	1:A:469:ARG:N	2.75	0.43
1:A:519:ARG:O	1:A:520:CYS:C	2.58	0.43
1:A:593:CYS:O	1:A:597:LYS:HG2	2.19	0.43
1:A:609:VAL:HG11	1:A:617:CYS:SG	2.58	0.43
1:A:518:PHE:O	1:A:521:LEU:HB3	2.18	0.43
1:A:352:ARG:HD2	1:A:352:ARG:C	2.43	0.43
1:A:463:MET:HE1	1:A:479:PHE:HE2	1.82	0.43
1:A:333:ASP:O	1:A:334:PRO:C	2.61	0.43
1:A:7:ARG:HG3	1:A:7:ARG:NH1	2.27	0.43
1:A:335:LEU:O	1:A:336:GLN:HG3	2.19	0.43
1:A:4:LYS:O	1:A:35:PRO:HA	2.19	0.43
1:A:51:ALA:HB1	1:A:56:GLU:HB2	2.01	0.42
1:A:381:ILE:O	1:A:587:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:GLY:HA2	1:A:587:ARG:NH1	2.34	0.42
1:A:144:LYS:HA	1:A:145:PRO:HA	1.88	0.42
1:A:383:ASN:O	1:A:383:ASN:CG	2.62	0.42
1:A:453:VAL:O	1:A:454:ASP:HB2	2.18	0.42
1:A:416:ASP:O	1:A:419:LYS:HG2	2.19	0.42
1:A:474:ARG:HE	1:A:477:GLU:CD	2.25	0.42
1:A:206:LYS:HZ3	1:A:296:LYS:CE	2.33	0.42
1:A:461:ILE:N	1:A:462:PRO:HD2	2.34	0.42
1:A:514:TYR:CE2	1:A:629:ARG:HD2	2.55	0.42
1:A:230:ASN:HA	5:A:930:HOH:O	2.20	0.42
1:A:347:LEU:O	1:A:348:GLY:C	2.63	0.42
1:A:456:THR:HG23	1:A:652:TYR:CE1	2.54	0.42
1:A:615:LYS:HG2	1:A:616:PHE:H	1.85	0.42
1:A:502:VAL:O	1:A:503:CYS:CB	2.66	0.41
1:A:443:LEU:O	1:A:444:GLU:C	2.63	0.41
1:A:447:LYS:NZ	1:A:526:ASP:OD2	2.53	0.41
1:A:51:ALA:O	1:A:56:GLU:N	2.53	0.41
1:A:286:SER:O	1:A:287:SER:HB2	2.21	0.41
1:A:206:LYS:HZ3	1:A:296:LYS:NZ	2.16	0.40
1:A:373:THR:HB	1:A:374:PRO:HD2	2.03	0.40
1:A:68:HIS:HB2	1:A:315:LEU:CD1	2.51	0.40
1:A:498:VAL:CG2	1:A:499:GLY:N	2.84	0.40
1:A:598:LEU:HA	1:A:598:LEU:HD23	1.87	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	672/676 (99%)	614 (91%)	48 (7%)	10 (2%)	8 18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	34	GLY
1	A	334	PRO
1	A	348	GLY
1	A	489	LYS
1	A	499	GLY
1	A	595	LYS
1	A	337	ASP
1	A	493	LEU
1	A	360	VAL

5.3.2 Protein sidechains [i](#)

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	566/571 (99%)	518 (92%)	48 (8%)	10	22

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	46	LEU
1	A	88	LYS
1	A	89	GLU
1	A	103	LYS
1	A	143	ARG
1	A	148	LYS
1	A	182	VAL
1	A	183	GLN
1	A	189	SER
1	A	240	GLN
1	A	260	GLU
1	A	304	LYS
1	A	313	LEU
1	A	321	THR
1	A	324	ARG
1	A	328	GLU

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Mol	Chain	Res	Type
1	A	331	CYS
1	A	333	ASP
1	A	335	LEU
1	A	336	GLN
1	A	338	GLU
1	A	340	LYS
1	A	343	LYS
1	A	352	ARG
1	A	359	SER
1	A	362	SER
1	A	372	GLU
1	A	377	CYS
1	A	383	ASN
1	A	418	LYS
1	A	434	SER
1	A	453	VAL
1	A	480	ARG
1	A	488	GLN
1	A	536	LEU
1	A	568	VAL
1	A	586	SER
1	A	596	GLN
1	A	597	LYS
1	A	608	THR
1	A	613	SER
1	A	623	THR
1	A	633	LYS
1	A	642	ASN
1	A	643	THR
1	A	661	LYS
1	A	675	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	312	ASN
1	A	349	HIS
1	A	481	GLN
1	A	572	HIS
1	A	642	ASN
1	A	676	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CO3	A	700	3	3,3,3	1.23	1 (33%)	2,3,3	0.86	0
2	CO3	A	701	3	3,3,3	1.20	1 (33%)	2,3,3	1.57	1 (50%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CO3	O1-C	2.02	1.32	1.25
2	A	700	CO3	O1-C	2.00	1.32	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CO3	O3-C-O1	2.08	125.00	119.68

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

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	674/676 (99%)	0.09	23 (3%)	48 42	21, 45, 76, 103	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	ASP	5.5
1	A	334	PRO	5.3
1	A	142	PRO	4.2
1	A	337	ASP	3.7
1	A	34	GLY	3.6
1	A	605	PHE	3.4
1	A	3	GLU	3.2
1	A	336	GLN	3.2
1	A	332	PRO	2.8
1	A	328	GLU	2.8
1	A	335	LEU	2.6
1	A	140	PRO	2.6
1	A	33	ASP	2.5
1	A	488	GLN	2.4
1	A	642	ASN	2.3
1	A	341	ALA	2.3
1	A	327	ARG	2.2
1	A	338	GLU	2.2
1	A	616	PHE	2.1
1	A	329	GLY	2.1
1	A	606	GLY	2.1
1	A	364	GLY	2.0
1	A	603	VAL	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	CO3	A	701	4/4	0.98	0.07	26,27,28,28	0
2	CO3	A	700	4/4	0.99	0.06	24,26,26,27	0
4	CL	A	800	1/1	0.99	0.08	24,24,24,24	0
3	FE	A	703	1/1	1.00	0.01	32,32,32,32	0
3	FE	A	702	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.