



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:50 AM UTC

PDB ID : 6Z8I / pdb_00006z8i
Title : Fructo-oligosaccharide transporter BT 1762-63
Authors : van den Berg, B.
Deposited on : 2020-06-02
Resolution : 2.62 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

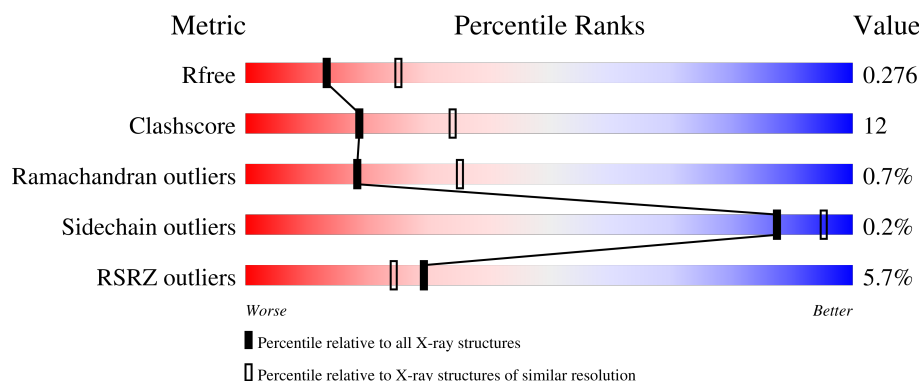
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	580	4% 73% 22% 5%
2	B	1041	5% 56% 21% 22%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10948 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 SusD homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	4447	2816	738	872	21	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	ALA	-	expression tag	UNP Q8A6W4
A	554	ALA	-	expression tag	UNP Q8A6W4
A	555	ALA	-	expression tag	UNP Q8A6W4
A	556	ALA	-	expression tag	UNP Q8A6W4
A	557	HIS	-	expression tag	UNP Q8A6W4
A	558	HIS	-	expression tag	UNP Q8A6W4
A	559	HIS	-	expression tag	UNP Q8A6W4
A	560	HIS	-	expression tag	UNP Q8A6W4
A	561	HIS	-	expression tag	UNP Q8A6W4
A	562	HIS	-	expression tag	UNP Q8A6W4

- Molecule 2 is a protein called SusC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	807	6414	4062	1090	1243	19	0	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

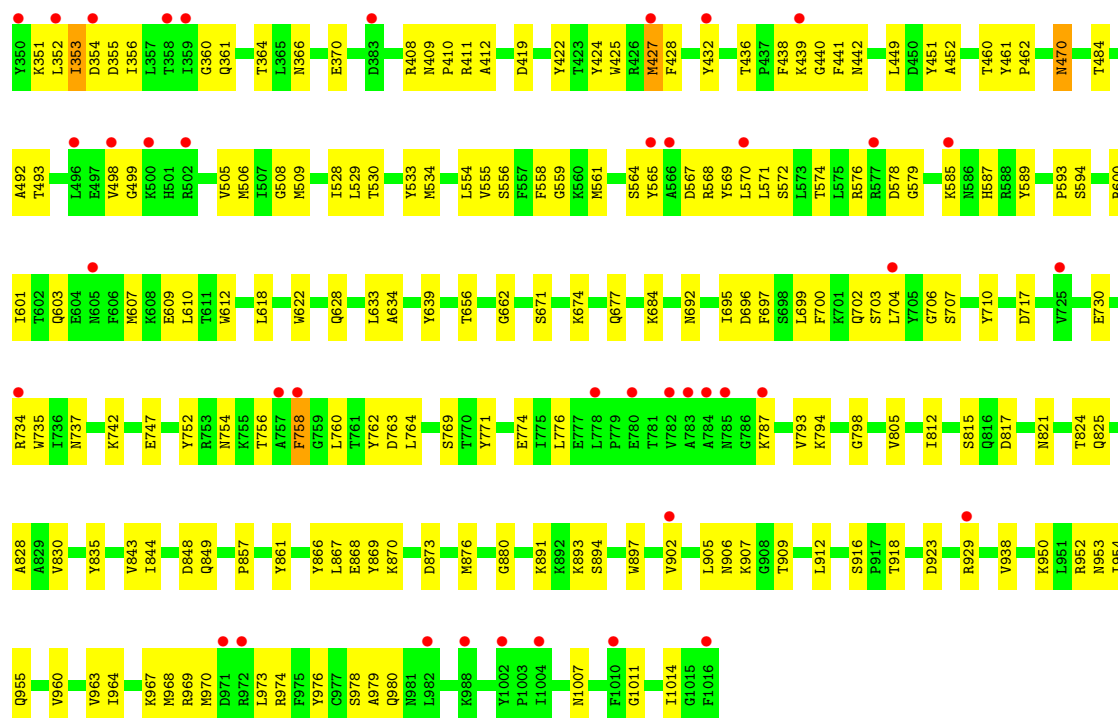
- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		
5	B	37	Total	O	0	0
			37	37		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	115.71Å 232.75Å 171.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.63 – 2.62 85.63 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.7 (85.63-2.62) 99.9 (85.63-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.62Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.217 , 0.275 0.220 , 0.276	Depositor DCC
R_{free} test set	3585 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10948	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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	0.39	0/4553	0.58	0/6178
2	B	0.40	1/6579 (0.0%)	0.63	2/8919 (0.0%)
All	All	0.40	1/11132 (0.0%)	0.61	2/15097 (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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	427	MET	CG-SD	-6.12	1.65	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	MET	CA-CB-CG	-5.44	103.22	114.10
2	B	969	ARG	CA-CB-CG	5.06	124.22	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	470	ASN	Peptide

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	4447	0	4216	100	0
2	B	6414	0	6079	160	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
5	A	43	0	0	6	0
5	B	37	0	0	6	0
All	All	10948	0	10295	252	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 12.

All (252) 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:445:MET:HE3	1:A:446:LEU:HD11	1.37	1.02
2:B:228:LYS:NZ	2:B:229:MET:O	1.97	0.97
2:B:228:LYS:HD2	2:B:229:MET:O	1.68	0.93
2:B:461:TYR:HE2	2:B:534:MET:HE1	1.35	0.89
1:A:445:MET:HG2	1:A:446:LEU:HD12	1.54	0.88
2:B:228:LYS:HZ1	2:B:230:ASN:HA	1.38	0.86
1:A:288:MET:HE2	1:A:381:GLU:HG3	1.57	0.84
2:B:461:TYR:CE2	2:B:534:MET:HE1	2.12	0.84
2:B:228:LYS:NZ	2:B:230:ASN:HA	1.94	0.82
1:A:536:PHE:HZ	2:B:793:VAL:HG12	1.44	0.81
1:A:437:ARG:NH2	5:A:702:HOH:O	2.07	0.81
1:A:19:ILE:HD12	2:B:639:TYR:CG	2.16	0.80
2:B:787:LYS:NZ	5:B:1201:HOH:O	2.16	0.78
1:A:20:ALA:O	5:A:701:HOH:O	2.00	0.78
1:A:32:ALA:HB3	1:A:126:MET:HE1	1.67	0.76
2:B:493:THR:HG22	2:B:506:MET:HG3	1.68	0.76
1:A:445:MET:HE3	1:A:446:LEU:CD1	2.15	0.74
2:B:699:LEU:HD13	2:B:704:LEU:HD23	1.68	0.74
2:B:505:VAL:HG12	2:B:561:MET:HG3	1.69	0.73
1:A:321:LEU:HB3	1:A:324:THR:HG23	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HD12	1:A:190:ILE:H	1.55	0.72
2:B:567:ASP:O	2:B:600:ARG:NH1	2.23	0.71
1:A:257:PHE:O	1:A:353:LYS:NZ	2.23	0.71
1:A:536:PHE:CZ	2:B:793:VAL:HG12	2.25	0.70
1:A:445:MET:HG2	1:A:446:LEU:CD1	2.21	0.70
2:B:963:VAL:HG23	2:B:964:ILE:HG13	1.71	0.70
1:A:84:ASP:HB2	1:A:87:ILE:HD12	1.76	0.68
1:A:445:MET:CE	1:A:446:LEU:HD11	2.20	0.67
1:A:82:THR:OG1	5:A:703:HOH:O	2.12	0.66
1:A:416:GLU:HG3	1:A:477:LEU:HD22	1.78	0.66
2:B:228:LYS:CD	2:B:229:MET:O	2.43	0.65
1:A:166:THR:OG1	5:A:704:HOH:O	2.15	0.65
2:B:228:LYS:NZ	2:B:231:VAL:H	1.95	0.65
2:B:346:MET:O	2:B:361:GLN:NE2	2.30	0.64
2:B:353:ILE:HG21	2:B:356:ILE:HD11	1.79	0.64
2:B:228:LYS:HZ1	2:B:231:VAL:H	1.45	0.64
2:B:756:THR:HG22	2:B:760:LEU:H	1.63	0.64
2:B:830:VAL:HG23	5:B:1205:HOH:O	1.98	0.63
2:B:873:ASP:OD2	2:B:974:ARG:NH1	2.31	0.63
1:A:494:ASP:OD1	1:A:497:ARG:NH2	2.32	0.63
1:A:14:VAL:HG12	1:A:18:GLN:HG3	1.81	0.62
2:B:411:ARG:NH2	5:B:1203:HOH:O	2.20	0.62
1:A:445:MET:CE	1:A:446:LEU:CD1	2.77	0.61
2:B:529:LEU:HA	2:B:534:MET:HE2	1.82	0.61
1:A:481:ARG:NH1	1:A:494:ASP:OD2	2.33	0.61
2:B:574:THR:HB	2:B:594:SER:OG	2.00	0.61
2:B:228:LYS:NZ	2:B:231:VAL:N	2.49	0.61
2:B:318:LYS:HA	2:B:351:LYS:HE2	1.82	0.60
2:B:955:GLN:HE21	2:B:976:TYR:HB2	1.66	0.60
2:B:794:LYS:HB2	2:B:805:VAL:HG21	1.82	0.60
2:B:825:GLN:HG2	2:B:828:ALA:HB2	1.84	0.59
1:A:203:TYR:O	1:A:207:THR:HG22	2.02	0.59
1:A:87:ILE:HG22	1:A:535:PRO:HG3	1.85	0.59
1:A:378:SER:O	1:A:382:ASN:ND2	2.32	0.59
1:A:473:ALA:HA	1:A:476:MET:HE2	1.85	0.59
2:B:228:LYS:NZ	2:B:230:ASN:CA	2.67	0.57
2:B:568:ARG:HD3	2:B:603:GLN:HB3	1.85	0.57
2:B:703:SER:O	2:B:752:TYR:HA	2.05	0.57
1:A:55:SER:O	5:A:705:HOH:O	2.18	0.57
1:A:32:ALA:CB	1:A:126:MET:HE1	2.34	0.57
2:B:699:LEU:HD13	2:B:704:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:451:TYR:CD2	2:B:484:THR:HG22	2.40	0.56
1:A:258:LEU:HB3	1:A:260:GLN:OE1	2.05	0.56
1:A:291:THR:HG21	1:A:381:GLU:OE1	2.05	0.56
2:B:228:LYS:HZ3	2:B:231:VAL:HG22	1.72	0.55
2:B:408:ARG:HG2	2:B:409:ASN:H	1.70	0.55
1:A:294:GLN:OE1	1:A:368:ARG:NH1	2.40	0.55
2:B:955:GLN:HG3	2:B:978:SER:HB3	1.88	0.55
2:B:953:ASN:OD1	2:B:980:GLN:NE2	2.40	0.54
1:A:171:TRP:HB3	1:A:211:LYS:HB2	1.90	0.54
1:A:213:TYR:HB3	1:A:222:LEU:HD21	1.90	0.54
2:B:364:THR:HG21	2:B:428:PHE:CZ	2.42	0.54
1:A:414:ARG:HG2	1:A:432:LEU:HD13	1.89	0.54
2:B:674:LYS:HE3	5:B:1206:HOH:O	2.08	0.54
2:B:893:LYS:NZ	2:B:906:ASN:O	2.40	0.54
2:B:232:LEU:HD22	2:B:236:GLN:HB3	1.90	0.53
2:B:825:GLN:HE22	2:B:835:TYR:HD1	1.56	0.53
2:B:979:ALA:HA	2:B:1007:ASN:O	2.08	0.53
1:A:111:MET:O	1:A:119:LYS:NZ	2.39	0.53
1:A:166:THR:HG23	1:A:169:GLU:H	1.73	0.53
2:B:869:TYR:CE2	2:B:870:LYS:HD3	2.44	0.53
1:A:369:SER:HB2	1:A:372:LEU:HB3	1.91	0.53
2:B:425:TRP:HB3	2:B:427:MET:HE1	1.91	0.53
2:B:976:TYR:CZ	2:B:1011:GLY:HA3	2.44	0.53
1:A:353:LYS:HE3	1:A:382:ASN:O	2.09	0.52
2:B:438:PHE:O	2:B:440:GLY:N	2.42	0.52
2:B:754:ASN:HB3	2:B:762:TYR:CE1	2.44	0.52
2:B:428:PHE:HA	2:B:449:LEU:O	2.09	0.52
2:B:812:ILE:HD11	2:B:923:ASP:O	2.09	0.52
1:A:260:GLN:H	1:A:260:GLN:CD	2.18	0.52
2:B:211:GLN:HB2	2:B:213:LYS:HE3	1.92	0.52
2:B:498:VAL:O	2:B:498:VAL:HG23	2.09	0.52
2:B:618:LEU:HD12	2:B:695:ILE:HG12	1.90	0.52
2:B:360:GLY:HA3	2:B:432:TYR:CZ	2.44	0.51
2:B:960:VAL:HG21	2:B:973:LEU:HD23	1.92	0.51
1:A:132:HIS:CE1	1:A:136:MET:HE2	2.46	0.51
2:B:891:LYS:HA	2:B:894:SER:OG	2.10	0.51
2:B:228:LYS:HZ1	2:B:231:VAL:N	2.07	0.51
2:B:462:PRO:HA	2:B:470:ASN:HD22	1.75	0.51
2:B:222:ALA:O	2:B:1007:ASN:HA	2.11	0.51
1:A:319:LYS:NZ	1:A:462:PRO:O	2.37	0.50
1:A:548:GLN:HG3	1:A:552:TRP:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:HA	1:A:75:GLU:OE1	2.11	0.50
1:A:403:ILE:HG21	1:A:406:ARG:HG2	1.93	0.50
2:B:242:TRP:O	2:B:246:VAL:HG22	2.11	0.50
2:B:866:TYR:O	2:B:867:LEU:HD23	2.12	0.50
2:B:334:ILE:O	2:B:337:THR:OG1	2.26	0.50
1:A:345:VAL:HG23	1:A:376:TYR:HB3	1.94	0.50
2:B:805:VAL:HG12	2:B:849:GLN:HB3	1.94	0.50
1:A:266:GLU:HG3	1:A:407:TYR:HB3	1.92	0.49
2:B:228:LYS:HZ2	2:B:229:MET:C	2.07	0.49
2:B:702:GLN:OE1	2:B:702:GLN:N	2.44	0.49
1:A:222:LEU:HD12	1:A:499:GLY:HA3	1.93	0.49
2:B:232:LEU:CD2	2:B:912:LEU:HD11	2.43	0.49
1:A:19:ILE:HD12	2:B:639:TYR:CD2	2.48	0.49
1:A:307:ASN:HB2	1:A:512:GLU:OE1	2.11	0.49
2:B:228:LYS:CE	2:B:229:MET:O	2.60	0.49
2:B:692:ASN:HA	2:B:710:TYR:O	2.13	0.49
1:A:172:GLN:OE1	1:A:211:LYS:HE2	2.13	0.49
2:B:763:ASP:C	2:B:764:LEU:HD23	2.38	0.49
2:B:530:THR:N	2:B:534:MET:HE2	2.28	0.48
1:A:211:LYS:HE3	1:A:229:ASP:OD1	2.12	0.48
2:B:756:THR:HG21	2:B:760:LEU:HB3	1.95	0.48
2:B:656:THR:O	2:B:671:SER:HA	2.13	0.48
2:B:968:MET:HB3	2:B:970:MET:HE3	1.96	0.48
2:B:587:HIS:CD2	2:B:684:LYS:HB3	2.49	0.48
1:A:33:TYR:OH	1:A:125:GLU:OE2	2.31	0.48
1:A:292:THR:HB	1:A:296:LEU:HD12	1.95	0.48
2:B:228:LYS:HZ1	2:B:230:ASN:CA	2.18	0.48
2:B:968:MET:HG2	2:B:970:MET:HE3	1.96	0.48
2:B:876:MET:HE3	2:B:954:ILE:HD12	1.95	0.47
2:B:506:MET:HE1	2:B:558:PHE:HD1	1.78	0.47
2:B:528:ILE:HB	2:B:533:TYR:CG	2.50	0.47
1:A:104:ALA:CB	1:A:126:MET:HE2	2.44	0.47
2:B:370:GLU:OE1	2:B:422:TYR:OH	2.26	0.47
1:A:66:GLU:OE1	1:A:66:GLU:N	2.41	0.47
2:B:259:TYR:CE2	2:B:276:MET:HE3	2.50	0.47
2:B:343:SER:OG	2:B:366:ASN:OD1	2.26	0.47
2:B:774:GLU:OE2	2:B:798:GLY:HA2	2.15	0.47
1:A:416:GLU:HG3	1:A:477:LEU:CD2	2.43	0.46
2:B:216:PHE:HD1	2:B:1014:ILE:CG2	2.28	0.46
2:B:756:THR:HG23	2:B:758:PHE:HB3	1.96	0.46
1:A:447:ILE:HG22	1:A:450:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ASP:OD2	2:B:411:ARG:NH1	2.48	0.46
2:B:460:THR:OG1	5:B:1202:HOH:O	2.20	0.46
2:B:634:ALA:HA	2:B:735:TRP:CD1	2.51	0.46
1:A:381:GLU:OE2	1:A:381:GLU:N	2.48	0.46
1:A:19:ILE:HD11	1:A:28:LEU:HD21	1.98	0.46
2:B:964:ILE:O	2:B:967:LYS:HB2	2.16	0.46
1:A:340:ARG:NH2	1:A:480:GLU:OE2	2.49	0.46
1:A:388:ASP:OD1	1:A:388:ASP:N	2.34	0.46
2:B:844:ILE:HA	2:B:848:ASP:OD1	2.16	0.46
1:A:441:ALA:HB2	1:A:460:VAL:HB	1.98	0.45
2:B:509:MET:HA	2:B:556:SER:O	2.16	0.45
2:B:554:LEU:HD23	2:B:579:GLY:O	2.16	0.45
2:B:570:LEU:HD12	2:B:571:LEU:H	1.81	0.45
2:B:909:THR:O	2:B:912:LEU:HD12	2.16	0.45
1:A:516:CYS:SG	1:A:518:ILE:HG12	2.55	0.45
1:A:437:ARG:HD3	1:A:461:THR:O	2.16	0.45
1:A:518:ILE:HG13	1:A:519:TYR:N	2.31	0.45
2:B:352:LEU:O	2:B:353:ILE:C	2.59	0.45
2:B:950:LYS:HE3	2:B:952:ARG:NH1	2.31	0.45
1:A:209:LEU:HD21	1:A:416:GLU:OE2	2.16	0.45
2:B:700:PHE:N	2:B:700:PHE:CD1	2.83	0.45
1:A:252:ASP:OD2	1:A:443:SER:HA	2.17	0.45
2:B:968:MET:HB2	2:B:968:MET:HE2	1.70	0.45
1:A:166:THR:CG2	1:A:169:GLU:H	2.29	0.45
2:B:408:ARG:HG2	2:B:409:ASN:N	2.31	0.45
2:B:601:ILE:HG22	2:B:607:MET:HG3	1.97	0.45
1:A:321:LEU:O	1:A:325:TYR:HB3	2.16	0.45
2:B:241:MET:HB2	2:B:897:TRP:CH2	2.52	0.45
2:B:700:PHE:N	2:B:700:PHE:HD1	2.15	0.45
1:A:124:ALA:HB1	1:A:181:ALA:HA	1.99	0.44
2:B:226:GLN:HG2	2:B:227:SER:N	2.32	0.44
2:B:609:GLU:HG3	2:B:609:GLU:O	2.15	0.44
1:A:253:TYR:H	1:A:443:SER:HB3	1.82	0.44
2:B:235:GLU:HA	2:B:276:MET:HE1	1.99	0.44
2:B:419:ASP:HB2	5:B:1216:HOH:O	2.17	0.44
1:A:317:GLN:O	1:A:461:THR:OG1	2.30	0.44
1:A:535:PRO:HB2	1:A:538:GLN:HG2	1.99	0.44
2:B:633:LEU:O	2:B:677:GLN:NE2	2.50	0.44
2:B:867:LEU:O	2:B:873:ASP:HA	2.18	0.44
2:B:279:SER:HB2	2:B:281:TYR:O	2.18	0.44
1:A:22:PRO:HA	1:A:111:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:742:LYS:HE2	2:B:776:LEU:HD21	1.98	0.44
2:B:861:TYR:CZ	2:B:880:GLY:HA3	2.53	0.44
1:A:5:LEU:HD11	2:B:555:VAL:HG12	1.98	0.44
1:A:472:GLU:O	1:A:476:MET:HG3	2.18	0.44
1:A:418:LEU:HB2	1:A:429:ALA:HB2	2.00	0.44
2:B:409:ASN:HB3	2:B:412:ALA:HB3	1.99	0.44
2:B:529:LEU:C	2:B:534:MET:HE2	2.43	0.44
2:B:612:TRP:H	2:B:612:TRP:CD1	2.35	0.44
2:B:628:GLN:HE21	2:B:628:GLN:HB3	1.61	0.44
2:B:295:TRP:CZ3	2:B:410:PRO:HD2	2.53	0.43
1:A:76:ILE:HG13	1:A:78:LYS:H	1.83	0.43
2:B:301:ARG:HD3	2:B:335:LYS:HG2	2.00	0.43
2:B:436:THR:HG23	2:B:441:PHE:O	2.19	0.43
1:A:66:GLU:OE2	2:B:929:ARG:HD2	2.18	0.43
2:B:610:LEU:HD22	2:B:612:TRP:HE1	1.82	0.43
2:B:508:GLY:HA3	2:B:558:PHE:CE1	2.53	0.43
1:A:77:SER:HA	1:A:80:ILE:HD11	2.01	0.43
2:B:281:TYR:HA	2:B:289:PRO:HA	1.99	0.43
2:B:771:TYR:CE1	2:B:857:PRO:HD2	2.53	0.43
1:A:340:ARG:HD2	1:A:483:VAL:O	2.19	0.43
2:B:717:ASP:HB3	2:B:737:ASN:HB3	2.00	0.42
1:A:214:ARG:O	1:A:222:LEU:HD23	2.19	0.42
1:A:406:ARG:NH2	1:A:488:GLU:OE1	2.47	0.42
1:A:96:GLN:HG2	2:B:730:GLU:N	2.35	0.42
1:A:338:ASP:OD1	1:A:340:ARG:NH1	2.52	0.42
2:B:824:THR:OG1	2:B:843:VAL:HG12	2.19	0.42
1:A:272:GLN:OE1	2:B:662:GLY:HA2	2.20	0.42
2:B:561:MET:O	2:B:572:SER:HA	2.20	0.42
1:A:17:ASP:OD1	1:A:17:ASP:N	2.48	0.42
1:A:210:TYR:HA	1:A:497:ARG:HD3	2.02	0.42
2:B:228:LYS:HD2	2:B:229:MET:C	2.39	0.42
2:B:235:GLU:HA	2:B:276:MET:CE	2.50	0.42
1:A:257:PHE:CZ	1:A:380:LYS:HE2	2.54	0.42
2:B:558:PHE:HB3	2:B:576:ARG:HG3	2.02	0.42
1:A:298:CYS:HA	1:A:299:CYS:HA	1.90	0.42
2:B:424:TYR:CE1	2:B:452:ALA:HB1	2.55	0.42
1:A:82:THR:HG22	1:A:533:PRO:HB2	2.02	0.41
1:A:414:ARG:HG2	1:A:432:LEU:CD1	2.49	0.41
2:B:506:MET:HE1	2:B:558:PHE:CD1	2.55	0.41
2:B:564:SER:HA	2:B:569:TYR:O	2.20	0.41
1:A:544:GLY:N	5:A:707:HOH:O	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:ILE:HB	2:B:356:ILE:HG13	2.02	0.41
2:B:902:VAL:HG13	2:B:905:LEU:HD11	2.03	0.41
2:B:578:ASP:O	2:B:589:TYR:HA	2.21	0.41
2:B:593:PRO:HG2	2:B:622:TRP:HZ3	1.86	0.41
2:B:229:MET:HE1	2:B:893:LYS:HG2	2.03	0.41
2:B:696:ASP:HA	2:B:707:SER:HA	2.03	0.41
2:B:916:SER:OG	2:B:918:THR:OG1	2.38	0.41
1:A:108:LEU:O	1:A:119:LYS:HE3	2.21	0.41
2:B:506:MET:O	2:B:559:GLY:HA2	2.20	0.41
2:B:451:TYR:HD2	2:B:484:THR:HG22	1.86	0.41
2:B:970:MET:HE2	2:B:970:MET:HB3	1.92	0.41
2:B:585:LYS:H	2:B:585:LYS:HD3	1.85	0.41
2:B:866:TYR:OH	2:B:868:GLU:OE1	2.34	0.41
1:A:52:ASP:CG	1:A:489:SER:HA	2.46	0.40
1:A:426:ILE:O	1:A:430:ILE:HG13	2.22	0.40
1:A:446:LEU:HD12	1:A:446:LEU:N	2.36	0.40
2:B:587:HIS:CG	2:B:684:LYS:HB3	2.55	0.40
2:B:906:ASN:O	2:B:907:LYS:HD3	2.21	0.40
1:A:152:MET:HG3	1:A:156:ALA:HB3	2.03	0.40
2:B:565:TYR:CD1	2:B:565:TYR:C	3.00	0.40
2:B:747:GLU:HG3	2:B:769:SER:HB3	2.04	0.40
2:B:817:ASP:O	2:B:821:ASN:HB2	2.21	0.40
2:B:530:THR:HG23	2:B:533:TYR:H	1.87	0.40
1:A:3:ASP:OD1	1:A:3:ASP:N	2.54	0.40
2:B:245:TYR:CD1	2:B:252:PRO:HA	2.56	0.40
2:B:442:ASN:O	2:B:492:ALA:HA	2.21	0.40
2:B:697:PHE:CZ	2:B:706:GLY:HA3	2.56	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	551/580 (95%)	524 (95%)	25 (4%)	2 (0%)	30	49
2	B	805/1041 (77%)	750 (93%)	48 (6%)	7 (1%)	14	28
All	All	1356/1621 (84%)	1274 (94%)	73 (5%)	9 (1%)	18	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	439	LYS
2	B	354	ASP
1	A	2	ASP
2	B	355	ASP
2	B	758	PHE
1	A	528	LYS
2	B	499	GLY
2	B	938	VAL
2	B	353	ILE

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	473/495 (96%)	473 (100%)	0	100	100
2	B	676/869 (78%)	674 (100%)	2 (0%)	86	94
All	All	1149/1364 (84%)	1147 (100%)	2 (0%)	87	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	734	ARG
2	B	815	SER

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	ASN
1	A	96	GLN
1	A	110	GLN
1	A	121	GLN
1	A	170	GLN
1	A	179	GLN
1	A	449	ASN
1	A	470	GLN
1	A	538	GLN
2	B	230	ASN
2	B	243	GLN
2	B	314	ASN
2	B	470	ASN
2	B	480	GLN
2	B	603	GLN
2	B	822	HIS
2	B	921	ASN
2	B	955	GLN
2	B	997	ASN

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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
4	PO4	A	602	-	4,4,4	1.08	0	6,6,6	0.53	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	553/580 (95%)	0.12	23 (4%)	40 35	35, 58, 85, 111	0
2	B	807/1041 (77%)	0.43	55 (6%)	23 19	37, 67, 106, 137	0
All	All	1360/1621 (83%)	0.30	78 (5%)	29 24	35, 63, 98, 137	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	CYS	4.9
2	B	211	GLN	4.8
2	B	780	GLU	4.5
2	B	358	THR	3.9
2	B	359	ILE	3.9
1	A	553	ALA	3.9
2	B	565	TYR	3.8
2	B	500	LYS	3.5
2	B	784	ALA	3.5
2	B	314	ASN	3.4
2	B	758	PHE	3.4
2	B	227	SER	3.3
2	B	566	ALA	3.3
2	B	427	MET	3.3
2	B	229	MET	3.3
2	B	1016	PHE	3.2
2	B	971	ASP	3.2
1	A	67	ASP	3.0
2	B	785	ASN	3.0
2	B	585	LYS	2.9
2	B	250	GLU	2.9
2	B	210	GLY	2.9
2	B	350	TYR	2.9
2	B	228	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	65	THR	2.8
2	B	212	ILE	2.7
2	B	352	LEU	2.7
2	B	577	ARG	2.7
2	B	605	ASN	2.7
1	A	59	TYR	2.6
2	B	734	ARG	2.6
1	A	63	SER	2.6
2	B	496	LEU	2.6
1	A	3	ASP	2.6
2	B	349	ASP	2.6
2	B	383	ASP	2.6
2	B	704	LEU	2.6
1	A	61	GLY	2.6
2	B	1004	ILE	2.5
2	B	313	SER	2.5
1	A	373	TYR	2.5
1	A	371	GLY	2.5
2	B	778	LEU	2.5
2	B	757	ALA	2.5
1	A	58	CYS	2.5
1	A	372	LEU	2.5
2	B	982	LEU	2.5
2	B	1002	TYR	2.5
2	B	498	VAL	2.5
1	A	492	PHE	2.4
1	A	447	ILE	2.4
1	A	388	ASP	2.4
1	A	60	LYS	2.4
2	B	787	LYS	2.3
1	A	450	TYR	2.3
2	B	988	LYS	2.3
2	B	902	VAL	2.3
2	B	342	PHE	2.3
2	B	1010	PHE	2.3
1	A	304	PRO	2.2
1	A	73	ALA	2.2
2	B	224	MET	2.2
2	B	256	ALA	2.2
1	A	516	CYS	2.2
2	B	972	ARG	2.2
2	B	570	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2	ASP	2.2
1	A	295	ILE	2.2
2	B	782	VAL	2.2
1	A	448	PHE	2.2
2	B	783	ALA	2.1
2	B	929	ARG	2.1
2	B	354	ASP	2.1
2	B	267	ALA	2.1
2	B	725	VAL	2.1
2	B	502	ARG	2.1
2	B	432	TYR	2.1
2	B	439	LYS	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
4	PO4	A	602	5/5	0.90	0.14	72,73,76,78	0
3	MG	B	1101	1/1	0.97	0.13	48,48,48,48	0
3	MG	A	601	1/1	0.97	0.25	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.