



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2017 – 09:40 PM EST

PDB ID : 5T3R
Title : Crystal structure of BT1762-1763
Authors : van den Berg, B.
Deposited on : 2016-08-26
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

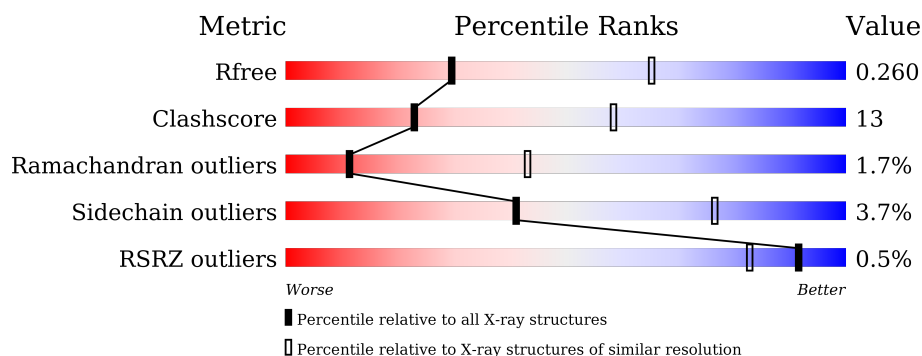
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	576	
2	D	1041	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	601	-	-	-	X
3	MG	D	1101	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10860 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
1	A	553	Total	C	N	O	S	0	1	0
			4455	2821	740	873	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	HIS	-	expression tag	UNP Q8A6W4
A	554	HIS	-	expression tag	UNP Q8A6W4
A	555	HIS	-	expression tag	UNP Q8A6W4
A	556	HIS	-	expression tag	UNP Q8A6W4
A	557	HIS	-	expression tag	UNP Q8A6W4
A	558	HIS	-	expression tag	UNP Q8A6W4

- Molecule 2 is a protein called SusC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	806	Total	C	N	O	S	0	0	0
			6402	4055	1088	1240	19			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

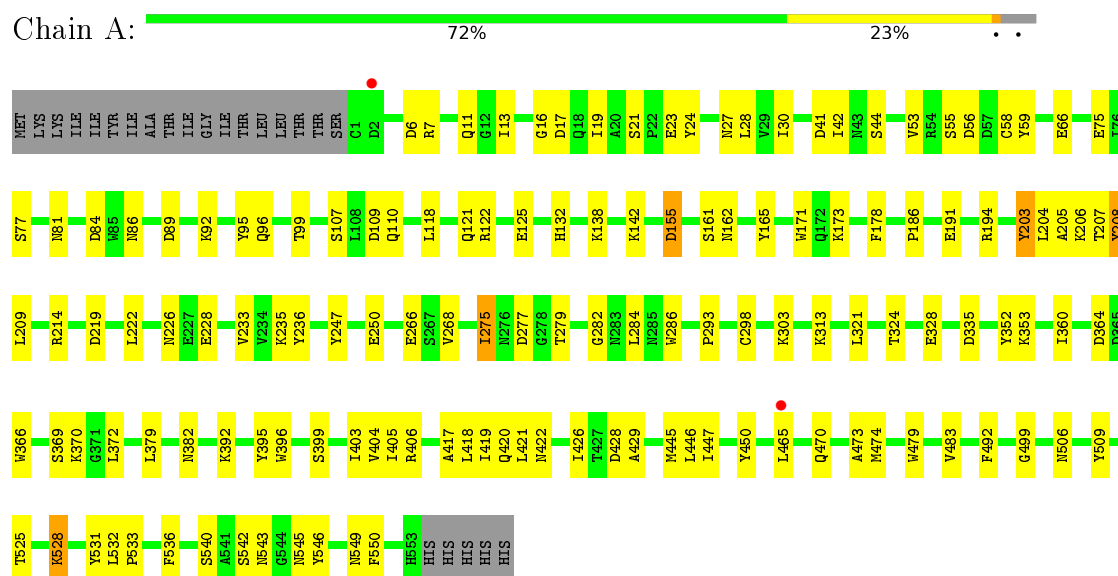
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

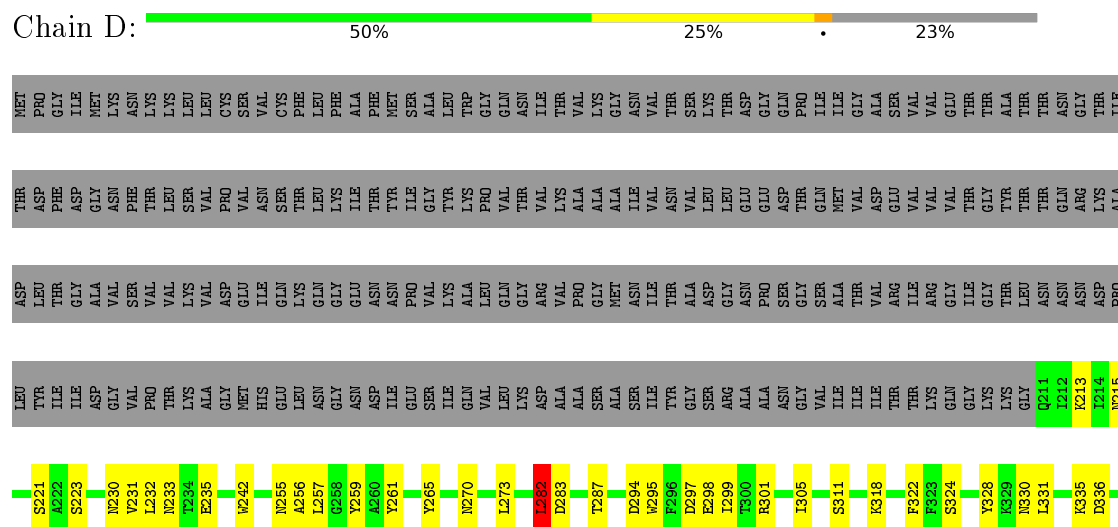
3 Residue-property plots

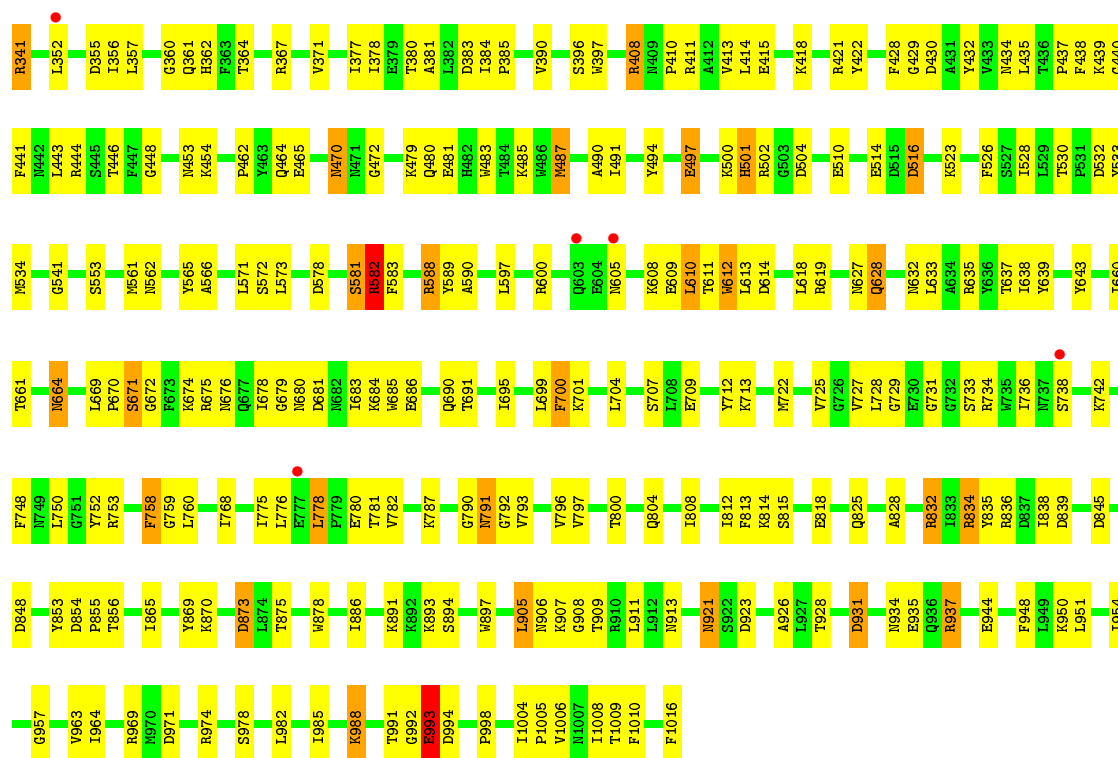
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: SusD homolog



• Molecule 2: SusC homolog





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.77Å 117.33Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.89 – 3.10 75.89 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.89-3.10) 99.9 (75.89-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.197 , 0.259 0.194 , 0.260	Depositor DCC
R_{free} test set	2067 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10860	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: NA, 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	0.47	0/4565	0.66	1/6194 (0.0%)
2	D	0.55	0/6567	0.78	4/8904 (0.0%)
All	All	0.52	0/11132	0.73	5/15098 (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	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	582	ARG	NE-CZ-NH2	-15.16	112.72	120.30
1	A	275	ILE	CG1-CB-CG2	-7.07	95.84	111.40
2	D	282	LEU	CA-CB-CG	6.43	130.09	115.30
2	D	778	LEU	CA-CB-CG	6.11	129.34	115.30
2	D	905	LEU	CA-CB-CG	5.71	128.42	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	582	ARG	Sidechain

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	4455	0	4222	98	0
2	D	6402	0	6055	205	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
All	All	10860	0	10277	285	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 13.

All (285) 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:178:PHE:CZ	1:A:203:TYR:CD2	2.11	1.39
1:A:178:PHE:CZ	1:A:203:TYR:CE2	2.30	1.19
1:A:178:PHE:CE1	1:A:203:TYR:HD2	1.63	1.15
1:A:178:PHE:CE1	1:A:203:TYR:CD2	2.43	1.03
1:A:178:PHE:HZ	1:A:203:TYR:CE2	1.78	0.90
2:D:832:ARG:NH1	2:D:935:GLU:OE2	2.08	0.87
1:A:370:LYS:HG3	2:D:256:ALA:HA	1.60	0.83
2:D:619:ARG:NH2	2:D:709:GLU:OE2	2.13	0.81
2:D:301:ARG:HG3	2:D:335:LYS:HG2	1.61	0.81
2:D:523:LYS:NZ	2:D:541:GLY:O	2.16	0.78
2:D:611:THR:O	2:D:613:LEU:N	2.16	0.77
1:A:178:PHE:CE2	1:A:203:TYR:CD2	2.73	0.76
2:D:504:ASP:HB2	2:D:562:ASN:HB2	1.67	0.74
2:D:528:ILE:HG22	2:D:530:THR:HG22	1.70	0.73
2:D:582:ARG:NH1	2:D:632:ASN:OD1	2.22	0.73
1:A:321:LEU:HB3	1:A:324:THR:HG23	1.73	0.70
1:A:277:ASP:OD1	1:A:279:THR:OG1	2.09	0.70
2:D:582:ARG:NE	2:D:628:GLN:OE1	2.24	0.70
1:A:178:PHE:HZ	1:A:203:TYR:HE2	1.39	0.69
2:D:699:LEU:HB2	2:D:704:LEU:HB3	1.73	0.69
2:D:377:ILE:HD13	2:D:414:LEU:HD21	1.74	0.68
1:A:204:LEU:HD12	1:A:204:LEU:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:894:SER:HA	2:D:908:GLY:HA3	1.75	0.68
2:D:748:PHE:HE2	2:D:750:LEU:HB2	1.60	0.67
2:D:691:THR:HG23	2:D:712:TYR:HB3	1.76	0.67
2:D:500:LYS:O	2:D:501:HIS:ND1	2.28	0.67
2:D:298:GLU:HG2	2:D:390:VAL:HG21	1.77	0.67
2:D:808:ILE:HG23	2:D:836:ARG:HG2	1.79	0.65
1:A:420:GLN:NE2	1:A:474:MET:SD	2.70	0.64
2:D:791:ASN:OD1	2:D:804:GLN:HG2	1.96	0.64
2:D:839:ASP:N	2:D:848:ASP:OD2	2.27	0.64
2:D:221:SER:HB3	2:D:305:ILE:HB	1.77	0.64
2:D:791:ASN:HD21	2:D:804:GLN:HE21	1.45	0.64
2:D:742:LYS:HB2	2:D:776:LEU:HD11	1.80	0.64
2:D:383:ASP:HB2	2:D:905:LEU:HB3	1.79	0.64
1:A:282:GLY:HA3	1:A:284:LEU:HD13	1.81	0.63
2:D:963:VAL:HG23	2:D:964:ILE:HG23	1.79	0.63
2:D:913:ASN:O	2:D:913:ASN:ND2	2.31	0.62
2:D:434:ASN:HA	2:D:444:ARG:HB2	1.82	0.62
2:D:671:SER:OG	2:D:672:GLY:N	2.33	0.62
1:A:540:SER:OG	2:D:792:GLY:O	2.11	0.62
2:D:432:TYR:HB3	2:D:446:THR:HB	1.81	0.61
1:A:205:ALA:O	1:A:206:LYS:C	2.38	0.61
2:D:873:ASP:HB3	2:D:957:GLY:O	2.00	0.61
1:A:277:ASP:HB2	2:D:669:LEU:HD11	1.84	0.60
1:A:542:SER:O	1:A:545:ASN:ND2	2.34	0.60
2:D:835:TYR:CE1	2:D:937:ARG:HD3	2.37	0.60
1:A:275:ILE:HG23	1:A:399:SER:HB3	1.82	0.59
2:D:609:GLU:O	2:D:611:THR:N	2.35	0.59
2:D:923:ASP:OD1	2:D:923:ASP:N	2.32	0.59
1:A:118:LEU:HD22	1:A:121:GLN:OE1	2.03	0.59
2:D:383:ASP:HB3	2:D:893:LYS:NZ	2.18	0.59
2:D:443:LEU:HD23	2:D:443:LEU:H	1.67	0.59
2:D:295:TRP:CD1	2:D:384:ILE:HG23	2.39	0.58
1:A:205:ALA:O	1:A:208:TYR:N	2.37	0.58
1:A:209:LEU:HD13	1:A:233:VAL:HG11	1.86	0.58
1:A:275:ILE:HG22	1:A:284:LEU:CD1	2.33	0.58
2:D:561:MET:HG2	2:D:573:LEU:HD12	1.87	0.57
2:D:561:MET:HB3	2:D:573:LEU:H	1.69	0.57
1:A:536:PHE:HZ	2:D:793:VAL:HG12	1.69	0.57
1:A:369:SER:HB2	1:A:372:LEU:HB3	1.86	0.56
1:A:293:PRO:HG3	1:A:352:TYR:CZ	2.40	0.56
1:A:30:ILE:HD13	2:D:670:PRO:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:760:LEU:HD12	2:D:869:TYR:HB2	1.86	0.56
2:D:362:HIS:HB2	2:D:430:ASP:OD1	2.06	0.56
2:D:383:ASP:HB3	2:D:893:LYS:HZ1	1.70	0.56
2:D:815:SER:HB3	2:D:818:GLU:HG3	1.88	0.55
1:A:53:VAL:HA	1:A:58:CYS:SG	2.45	0.55
2:D:360:GLY:HA3	2:D:432:TYR:CZ	2.41	0.55
2:D:242:TRP:HB2	2:D:261:TYR:CZ	2.41	0.55
2:D:377:ILE:O	2:D:380:THR:HG22	2.07	0.55
2:D:825:GLN:HB3	2:D:828:ALA:HB2	1.89	0.55
2:D:893:LYS:NZ	2:D:906:ASN:O	2.40	0.55
2:D:462:PRO:HB3	2:D:472:GLY:HA2	1.87	0.55
2:D:690:GLN:HB2	2:D:713:LYS:HG2	1.89	0.55
2:D:377:ILE:O	2:D:381:ALA:N	2.39	0.54
1:A:161:SER:OG	1:A:545:ASN:O	2.23	0.54
2:D:637:THR:HG22	2:D:678:ILE:HA	1.89	0.54
2:D:988:LYS:HD2	2:D:988:LYS:H	1.73	0.54
2:D:628:GLN:HB2	2:D:685:TRP:CZ3	2.43	0.54
2:D:778:LEU:HD12	2:D:782:VAL:HG12	1.90	0.54
2:D:736:ILE:HD13	2:D:738:SER:HB3	1.90	0.54
2:D:790:GLY:O	2:D:792:GLY:N	2.41	0.54
2:D:748:PHE:HB3	2:D:768:ILE:HG23	1.91	0.53
2:D:873:ASP:OD2	2:D:974:ARG:NH2	2.41	0.53
1:A:84:ASP:HB3	1:A:86:ASN:OD1	2.09	0.53
1:A:142:LYS:HD2	1:A:531:TYR:CE2	2.43	0.53
2:D:336:ASP:OD2	2:D:411:ARG:NH2	2.41	0.53
2:D:605:ASN:HA	2:D:608:LYS:HD2	1.90	0.53
2:D:838:ILE:N	2:D:848:ASP:OD2	2.42	0.53
2:D:232:LEU:HD22	2:D:907:LYS:O	2.08	0.52
1:A:275:ILE:HG22	1:A:284:LEU:HD11	1.91	0.52
2:D:589:TYR:O	2:D:590:ALA:HB3	2.08	0.52
2:D:583:PHE:O	2:D:588:ARG:NH1	2.42	0.52
2:D:832:ARG:NH2	2:D:928:THR:HG23	2.25	0.52
2:D:832:ARG:NH2	2:D:926:ALA:HB3	2.24	0.52
2:D:430:ASP:HA	2:D:448:GLY:HA2	1.91	0.52
2:D:633:LEU:HB3	2:D:638:ILE:HD11	1.91	0.52
2:D:439:LYS:HD2	2:D:440:GLY:N	2.25	0.52
2:D:470:ASN:ND2	2:D:470:ASN:O	2.41	0.52
2:D:384:ILE:HD12	2:D:385:PRO:HD2	1.91	0.52
2:D:610:LEU:O	2:D:612:TRP:CD1	2.62	0.52
1:A:353:LYS:NZ	1:A:382:ASN:O	2.37	0.51
2:D:813:PHE:CE1	2:D:834:ARG:HG3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:886:ILE:HD12	2:D:998:PRO:HG3	1.91	0.51
2:D:504:ASP:HB2	2:D:562:ASN:CB	2.38	0.51
2:D:832:ARG:HH22	2:D:926:ALA:C	2.14	0.51
2:D:362:HIS:O	2:D:429:GLY:HA3	2.10	0.51
1:A:313:LYS:HE3	1:A:335:ASP:OD2	2.11	0.51
2:D:637:THR:HG22	2:D:679:GLY:H	1.77	0.50
2:D:835:TYR:CZ	2:D:937:ARG:HD3	2.45	0.50
2:D:681:ASP:N	2:D:681:ASP:OD1	2.34	0.50
2:D:335:LYS:O	2:D:414:LEU:HD13	2.10	0.50
2:D:674:LYS:HE2	2:D:676:ASN:OD1	2.11	0.50
2:D:618:LEU:HD23	2:D:695:ILE:HG13	1.92	0.50
2:D:553:SER:H	2:D:581:SER:HB3	1.76	0.50
2:D:230:ASN:O	2:D:909:THR:HB	2.11	0.50
2:D:532:ASP:OD1	2:D:532:ASP:N	2.44	0.50
2:D:853:TYR:OH	2:D:855:PRO:HB3	2.12	0.50
1:A:447:ILE:HG22	1:A:450:TYR:CZ	2.46	0.50
1:A:66:GLU:OE1	2:D:897:TRP:NE1	2.38	0.50
2:D:435:LEU:HG	2:D:437:PRO:HD3	1.93	0.49
2:D:578:ASP:O	2:D:589:TYR:HA	2.12	0.49
2:D:722:MET:HE1	2:D:787:LYS:HG2	1.94	0.49
2:D:483:TRP:HA	2:D:516:ASP:HB3	1.94	0.49
2:D:934:ASN:HD22	2:D:937:ARG:HB3	1.77	0.49
2:D:944:GLU:OE1	2:D:991:THR:HG23	2.13	0.49
1:A:419:ILE:HG12	1:A:473:ALA:HB1	1.94	0.49
1:A:525:THR:HG21	1:A:528:LYS:HD2	1.94	0.49
2:D:371:VAL:HG22	2:D:421:ARG:HB2	1.94	0.49
2:D:497:GLU:HB2	2:D:502:ARG:CD	2.42	0.49
2:D:583:PHE:HD1	2:D:683:ILE:HG23	1.77	0.49
1:A:55:SER:HB3	1:A:492:PHE:HB2	1.93	0.49
1:A:417:ALA:O	1:A:421:LEU:HG	2.12	0.49
1:A:422:ASN:ND2	1:A:470:GLN:HB2	2.28	0.49
2:D:1004:ILE:HD12	2:D:1005:PRO:HD2	1.95	0.49
2:D:232:LEU:HB2	2:D:906:ASN:HD21	1.78	0.49
1:A:250:GLU:HG2	1:A:266:GLU:HB2	1.94	0.49
2:D:796:VAL:O	2:D:796:VAL:HG12	2.13	0.49
1:A:418:LEU:HB2	1:A:429:ALA:HB2	1.95	0.48
2:D:352:LEU:HB2	2:D:357:LEU:HD12	1.94	0.48
2:D:832:ARG:HH21	2:D:928:THR:HG23	1.78	0.48
2:D:255:ASN:ND2	2:D:259:TYR:HB2	2.28	0.48
2:D:988:LYS:H	2:D:988:LYS:CD	2.26	0.48
1:A:132:HIS:HA	1:A:203:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:HG2	2:D:661:THR:HG22	1.95	0.48
2:D:854:ASP:OD1	2:D:856:THR:OG1	2.32	0.48
2:D:748:PHE:CE2	2:D:750:LEU:HB2	2.45	0.48
1:A:59:TYR:HA	1:A:75:GLU:OE2	2.14	0.48
2:D:408:ARG:NH2	2:D:465:GLU:OE2	2.38	0.48
2:D:891:LYS:HE3	2:D:991:THR:HG21	1.95	0.48
2:D:299:ILE:HG21	2:D:410:PRO:HB2	1.95	0.47
2:D:265:TYR:HA	2:D:270:ASN:O	2.15	0.47
2:D:526:PHE:CD2	2:D:534:MET:HG2	2.49	0.47
1:A:445:MET:HG2	1:A:446:LEU:HG	1.97	0.47
1:A:532:LEU:HB3	1:A:533:PRO:HD2	1.97	0.47
2:D:814:LYS:NZ	2:D:921:ASN:HA	2.30	0.47
2:D:800:THR:HG21	2:D:856:THR:HG23	1.97	0.47
2:D:415:GLU:O	2:D:418:LYS:HG2	2.15	0.47
2:D:725:VAL:HG13	2:D:728:LEU:HB2	1.97	0.47
2:D:408:ARG:HD3	2:D:413:VAL:HG23	1.97	0.47
2:D:690:GLN:OE1	2:D:713:LYS:HE3	2.15	0.47
1:A:125:GLU:OE1	1:A:194:ARG:NH2	2.37	0.46
1:A:284:LEU:HB2	1:A:286:TRP:CE2	2.50	0.46
2:D:341:ARG:HA	2:D:367:ARG:O	2.14	0.46
2:D:758:PHE:O	2:D:760:LEU:N	2.48	0.46
1:A:303:LYS:HB3	1:A:303:LYS:HE3	1.66	0.46
2:D:322:PHE:CE2	2:D:324:SER:HB2	2.51	0.46
2:D:235:GLU:OE1	2:D:235:GLU:CA	2.64	0.46
1:A:132:HIS:HA	1:A:203:TYR:HE2	1.79	0.46
1:A:19:ILE:HG13	2:D:639:TYR:CG	2.51	0.46
1:A:99:THR:OG1	2:D:729:GLY:HA3	2.16	0.46
2:D:780:GLU:OE1	2:D:781:THR:HG23	2.16	0.46
2:D:487:MET:HE2	2:D:510:GLU:OE1	2.16	0.46
1:A:21:SER:HB3	1:A:23:GLU:OE1	2.16	0.45
2:D:878:TRP:CZ2	2:D:951:LEU:HD12	2.51	0.45
2:D:582:ARG:O	2:D:635:ARG:HD3	2.16	0.45
2:D:700:PHE:CD1	2:D:700:PHE:N	2.77	0.45
1:A:404:VAL:HG12	1:A:405:ILE:HG13	1.96	0.45
1:A:138:LYS:HG2	1:A:171:TRP:CZ2	2.51	0.45
2:D:748:PHE:HB3	2:D:768:ILE:CG2	2.45	0.45
1:A:275:ILE:HD13	1:A:275:ILE:HG21	1.49	0.45
1:A:275:ILE:HG22	1:A:284:LEU:HD12	1.98	0.45
1:A:422:ASN:HA	1:A:426:ILE:HD11	1.98	0.45
1:A:16:GLY:HA3	2:D:637:THR:OG1	2.17	0.45
1:A:370:LYS:CG	2:D:256:ALA:HA	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:490:ALA:C	2:D:491:ILE:HG13	2.37	0.45
2:D:397:TRP:HZ2	2:D:415:GLU:HG3	1.80	0.45
2:D:364:THR:HB	2:D:428:PHE:CE1	2.52	0.45
2:D:480:GLN:HE21	2:D:481:GLU:H	1.64	0.45
2:D:780:GLU:N	2:D:780:GLU:OE2	2.47	0.45
1:A:56:ASP:OD1	1:A:56:ASP:N	2.48	0.45
2:D:328:TYR:CE1	2:D:330:ASN:HB2	2.52	0.45
1:A:138:LYS:HG2	1:A:171:TRP:CH2	2.52	0.45
1:A:403:ILE:HG21	1:A:406:ARG:HG2	1.99	0.45
2:D:223:SER:HA	2:D:1006:VAL:O	2.17	0.45
2:D:282:LEU:H	2:D:282:LEU:HD12	1.82	0.45
2:D:637:THR:CG2	2:D:679:GLY:H	2.29	0.45
2:D:748:PHE:CE2	2:D:750:LEU:HD12	2.52	0.45
1:A:275:ILE:CG2	1:A:399:SER:HB3	2.46	0.44
1:A:353:LYS:NZ	1:A:379:LEU:O	2.43	0.44
2:D:869:TYR:CE1	2:D:870:LYS:HG3	2.53	0.44
1:A:479:TRP:O	1:A:483:VAL:HG22	2.17	0.44
2:D:422:TYR:CD1	2:D:422:TYR:C	2.91	0.44
2:D:643:TYR:HD2	2:D:671:SER:HB2	1.83	0.44
1:A:42:ILE:HD13	1:A:395:TYR:CE2	2.52	0.44
2:D:612:TRP:HB2	2:D:700:PHE:CD1	2.53	0.44
2:D:894:SER:O	2:D:911:LEU:HB3	2.18	0.44
2:D:331:LEU:HD23	2:D:331:LEU:HA	1.78	0.44
1:A:121:GLN:HG2	1:A:186:PRO:HD3	1.99	0.44
2:D:294:ASP:O	2:D:297:ASP:N	2.49	0.44
2:D:441:PHE:HD1	2:D:494:TYR:HB2	1.83	0.44
2:D:675:ARG:HG2	2:D:731:GLY:HA3	2.00	0.44
1:A:219:ASP:HB3	1:A:550:PHE:CE1	2.53	0.43
2:D:257:LEU:N	2:D:257:LEU:HD23	2.34	0.43
2:D:231:VAL:HB	2:D:906:ASN:OD1	2.19	0.43
2:D:453:ASN:OD1	2:D:480:GLN:NE2	2.52	0.43
1:A:205:ALA:O	1:A:207:THR:N	2.52	0.43
2:D:500:LYS:HG3	2:D:566:ALA:HB2	1.99	0.43
2:D:954:ILE:O	2:D:978:SER:HA	2.18	0.43
2:D:479:LYS:HB3	2:D:479:LYS:HE3	1.85	0.43
2:D:712:TYR:CD1	2:D:712:TYR:O	2.72	0.43
1:A:107:SER:HA	1:A:110:GLN:HG2	2.00	0.43
1:A:235:LYS:HD3	1:A:236:TYR:CE2	2.52	0.43
2:D:530:THR:HG23	2:D:533:TYR:H	1.84	0.43
2:D:377:ILE:HA	2:D:380:THR:HG22	2.00	0.43
2:D:377:ILE:HG13	2:D:378:ILE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:934:ASN:ND2	2:D:937:ARG:HB3	2.34	0.43
1:A:19:ILE:HD12	1:A:28:LEU:HD21	2.00	0.43
2:D:221:SER:HA	2:D:1008:ILE:O	2.18	0.42
2:D:775:ILE:HG22	2:D:797:VAL:HA	2.00	0.42
2:D:485:LYS:HE2	2:D:514:GLU:OE1	2.18	0.42
1:A:214:ARG:HH21	1:A:226:ASN:CG	2.23	0.42
1:A:41:ASP:HB3	1:A:44:SER:OG	2.19	0.42
1:A:165:TYR:CE1	1:A:173:LYS:HE3	2.55	0.42
2:D:215:ASN:HB2	2:D:311:SER:OG	2.20	0.42
2:D:612:TRP:HB2	2:D:700:PHE:CE1	2.55	0.42
2:D:704:LEU:HD13	2:D:752:TYR:HD1	1.85	0.42
1:A:81:ASN:ND2	2:D:934:ASN:OD1	2.53	0.42
1:A:30:ILE:HD13	2:D:670:PRO:CB	2.50	0.42
2:D:950:LYS:HB2	2:D:950:LYS:HE2	1.89	0.42
1:A:11:GLN:O	1:A:13:ILE:HD12	2.20	0.42
2:D:221:SER:HB2	2:D:1009:THR:HG23	2.00	0.42
2:D:355:ASP:O	2:D:356:ILE:HD12	2.20	0.42
2:D:361:GLN:HG3	2:D:361:GLN:O	2.20	0.42
2:D:695:ILE:O	2:D:707:SER:HA	2.20	0.42
2:D:931:ASP:OD2	2:D:934:ASN:HA	2.19	0.42
2:D:948:PHE:HA	2:D:985:ILE:O	2.20	0.42
1:A:399:SER:OG	2:D:664:ASN:ND2	2.53	0.42
1:A:392:LYS:HD3	1:A:396:TRP:CD1	2.55	0.41
1:A:543:ASN:ND2	2:D:780:GLU:HB2	2.35	0.41
1:A:284:LEU:HD22	1:A:286:TRP:CZ2	2.55	0.41
1:A:506:ASN:O	1:A:509:TYR:HB2	2.20	0.41
2:D:643:TYR:CD2	2:D:671:SER:HB2	2.55	0.41
1:A:155:ASP:OD1	1:A:155:ASP:N	2.53	0.41
1:A:421:LEU:HA	1:A:421:LEU:HD23	1.75	0.41
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.86	0.41
1:A:30:ILE:HG12	2:D:660:ILE:HG13	2.02	0.41
2:D:758:PHE:HD1	2:D:758:PHE:H	1.67	0.41
2:D:992:GLY:O	2:D:993:GLU:HB2	2.20	0.41
2:D:230:ASN:HB2	2:D:909:THR:HG21	2.02	0.41
2:D:408:ARG:HD3	2:D:413:VAL:CG2	2.51	0.41
2:D:526:PHE:CG	2:D:534:MET:HG2	2.55	0.41
2:D:571:LEU:HD12	2:D:572:SER:N	2.35	0.41
2:D:242:TRP:HB2	2:D:261:TYR:CE1	2.56	0.41
2:D:242:TRP:CD2	2:D:273:LEU:HD13	2.55	0.41
2:D:812:ILE:HD11	2:D:923:ASP:O	2.21	0.41
1:A:360:ILE:HA	1:A:366:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:627:ASN:HB3	2:D:686:GLU:HB3	2.02	0.41
1:A:162:ASN:OD1	1:A:546:TYR:HA	2.20	0.41
2:D:298:GLU:HG2	2:D:390:VAL:CG2	2.50	0.41
1:A:222:LEU:HD13	1:A:499:GLY:HA3	2.03	0.40
2:D:256:ALA:C	2:D:257:LEU:HD23	2.42	0.40
2:D:283:ASP:OD2	2:D:287:THR:OG1	2.30	0.40
2:D:808:ILE:CG2	2:D:838:ILE:HD11	2.51	0.40
1:A:23:GLU:HG2	1:A:24:TYR:CD1	2.56	0.40
1:A:313:LYS:NZ	1:A:328:GLU:O	2.54	0.40
2:D:1010:PHE:N	2:D:1010:PHE:CD1	2.90	0.40
1:A:27:ASN:HB3	2:D:672:GLY:HA2	2.04	0.40
2:D:680:ASN:HB3	2:D:734:ARG:HH21	1.86	0.40
2:D:873:ASP:O	2:D:957:GLY:N	2.54	0.40
1:A:247:TYR:CE1	1:A:268:VAL:HA	2.56	0.40
1:A:92:LYS:O	1:A:96:GLN:HG3	2.21	0.40
1:A:95:TYR:CE1	2:D:727:VAL:HG12	2.56	0.40
2:D:865:ILE:O	2:D:875:THR:HA	2.21	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	552/576 (96%)	505 (92%)	44 (8%)	3 (0%)	34	72
2	D	804/1041 (77%)	691 (86%)	93 (12%)	20 (2%)	7	32
All	All	1356/1617 (84%)	1196 (88%)	137 (10%)	23 (2%)	11	43

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	501	HIS

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Mol	Chain	Res	Type
2	D	610	LEU
2	D	612	TRP
2	D	759	GLY
2	D	845	ASP
1	A	528	LYS
2	D	396	SER
2	D	438	PHE
2	D	971	ASP
2	D	282	LEU
2	D	318	LYS
2	D	700	PHE
2	D	733	SER
2	D	931	ASP
2	D	982	LEU
2	D	993	GLU
1	A	77	SER
1	A	465	LEU
2	D	233	ASN
2	D	758	PHE
2	D	791	ASN
2	D	581	SER
2	D	994	ASP

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	475/495 (96%)	462 (97%)	13 (3%)	52	82
2	D	673/869 (77%)	644 (96%)	29 (4%)	35	72
All	All	1148/1364 (84%)	1106 (96%)	42 (4%)	41	76

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP

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Mol	Chain	Res	Type
1	A	7	ARG
1	A	17	ASP
1	A	89	ASP
1	A	109	ASP
1	A	155	ASP
1	A	203	TYR
1	A	208	TYR
1	A	228	GLU
1	A	298	CYS
1	A	364	ASP
1	A	428	ASP
1	A	549	ASN
2	D	213	LYS
2	D	341	ARG
2	D	408	ARG
2	D	454	LYS
2	D	464	GLN
2	D	470	ASN
2	D	487	MET
2	D	497	GLU
2	D	516	ASP
2	D	565	TYR
2	D	588	ARG
2	D	597	LEU
2	D	600	ARG
2	D	614	ASP
2	D	628	GLN
2	D	664	ASN
2	D	671	SER
2	D	684	LYS
2	D	701	LYS
2	D	753	ARG
2	D	832	ARG
2	D	834	ARG
2	D	873	ASP
2	D	921	ASN
2	D	937	ARG
2	D	969	ARG
2	D	988	LYS
2	D	993	GLU
2	D	1016	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	110	GLN
2	D	233	ASN
2	D	236	GLN
2	D	243	GLN
2	D	247	ASN
2	D	804	GLN
2	D	906	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	553/576 (96%)	-0.43	2 (0%) 93 85	39, 76, 118, 164	0
2	D	806/1041 (77%)	-0.40	5 (0%) 90 80	34, 67, 125, 196	0
All	All	1359/1617 (84%)	-0.41	7 (0%) 91 83	34, 70, 122, 196	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASP	4.2
2	D	605	ASN	3.7
2	D	777	GLU	2.7
2	D	603	GLN	2.7
1	A	465	LEU	2.3
2	D	352	LEU	2.1
2	D	738	SER	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	A	601	1/1	0.96	0.29	4.41	53,53,53,53	0
3	MG	D	1101	1/1	0.97	0.23	2.10	45,45,45,45	0
4	NA	A	602	1/1	0.76	0.12	-1.03	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.