



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:39 pm BST

PDB ID : 3EI3
Title : Structure of the hsDDB1-drDDB2 complex
Authors : Scrima, A.; Thoma, N.H.
Deposited on : 2008-09-15
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

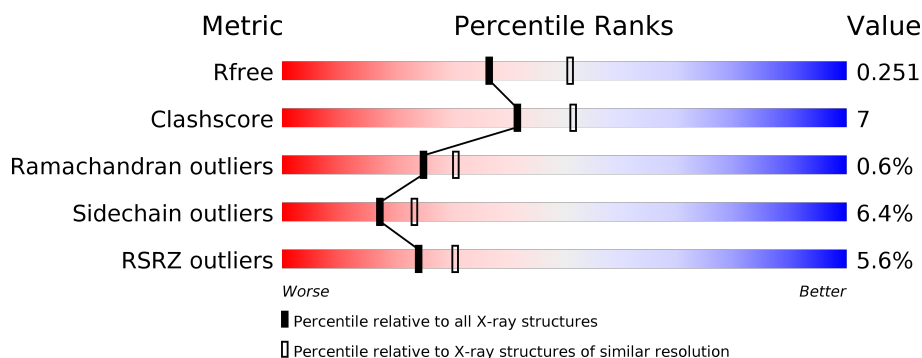
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	1158	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div> </div>
2	B	383	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12246 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1105	8693	5516	1462	1667	48	31	4	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	EXPRESSION TAG	UNP Q16531
A	-16	HIS	-	EXPRESSION TAG	UNP Q16531
A	-15	HIS	-	EXPRESSION TAG	UNP Q16531
A	-14	HIS	-	EXPRESSION TAG	UNP Q16531
A	-13	HIS	-	EXPRESSION TAG	UNP Q16531
A	-12	HIS	-	EXPRESSION TAG	UNP Q16531
A	-11	HIS	-	EXPRESSION TAG	UNP Q16531
A	-10	ARG	-	EXPRESSION TAG	UNP Q16531
A	-9	ARG	-	EXPRESSION TAG	UNP Q16531
A	-8	LEU	-	EXPRESSION TAG	UNP Q16531
A	-7	VAL	-	EXPRESSION TAG	UNP Q16531
A	-6	PRO	-	EXPRESSION TAG	UNP Q16531
A	-5	ARG	-	EXPRESSION TAG	UNP Q16531
A	-4	GLY	-	EXPRESSION TAG	UNP Q16531
A	-3	SER	-	EXPRESSION TAG	UNP Q16531
A	-2	GLY	-	EXPRESSION TAG	UNP Q16531
A	-1	GLY	-	EXPRESSION TAG	UNP Q16531
A	0	ARG	-	EXPRESSION TAG	UNP Q16531

- Molecule 2 is a protein called DNA damage-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	355	2843	1806	499	527	11	19	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	75	MET	-	EXPRESSION TAG	UNP Q2YDS1
B	76	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	77	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	78	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	79	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	80	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	81	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	82	VAL	-	EXPRESSION TAG	UNP Q2YDS1
B	83	ASP	-	EXPRESSION TAG	UNP Q2YDS1
B	84	GLU	-	EXPRESSION TAG	UNP Q2YDS1
B	85	ASN	-	EXPRESSION TAG	UNP Q2YDS1
B	86	LEU	-	EXPRESSION TAG	UNP Q2YDS1
B	87	TYR	-	EXPRESSION TAG	UNP Q2YDS1
B	88	PHE	-	EXPRESSION TAG	UNP Q2YDS1
B	89	GLN	-	EXPRESSION TAG	UNP Q2YDS1
B	90	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	91	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	92	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	93	ARG	-	EXPRESSION TAG	UNP Q2YDS1

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

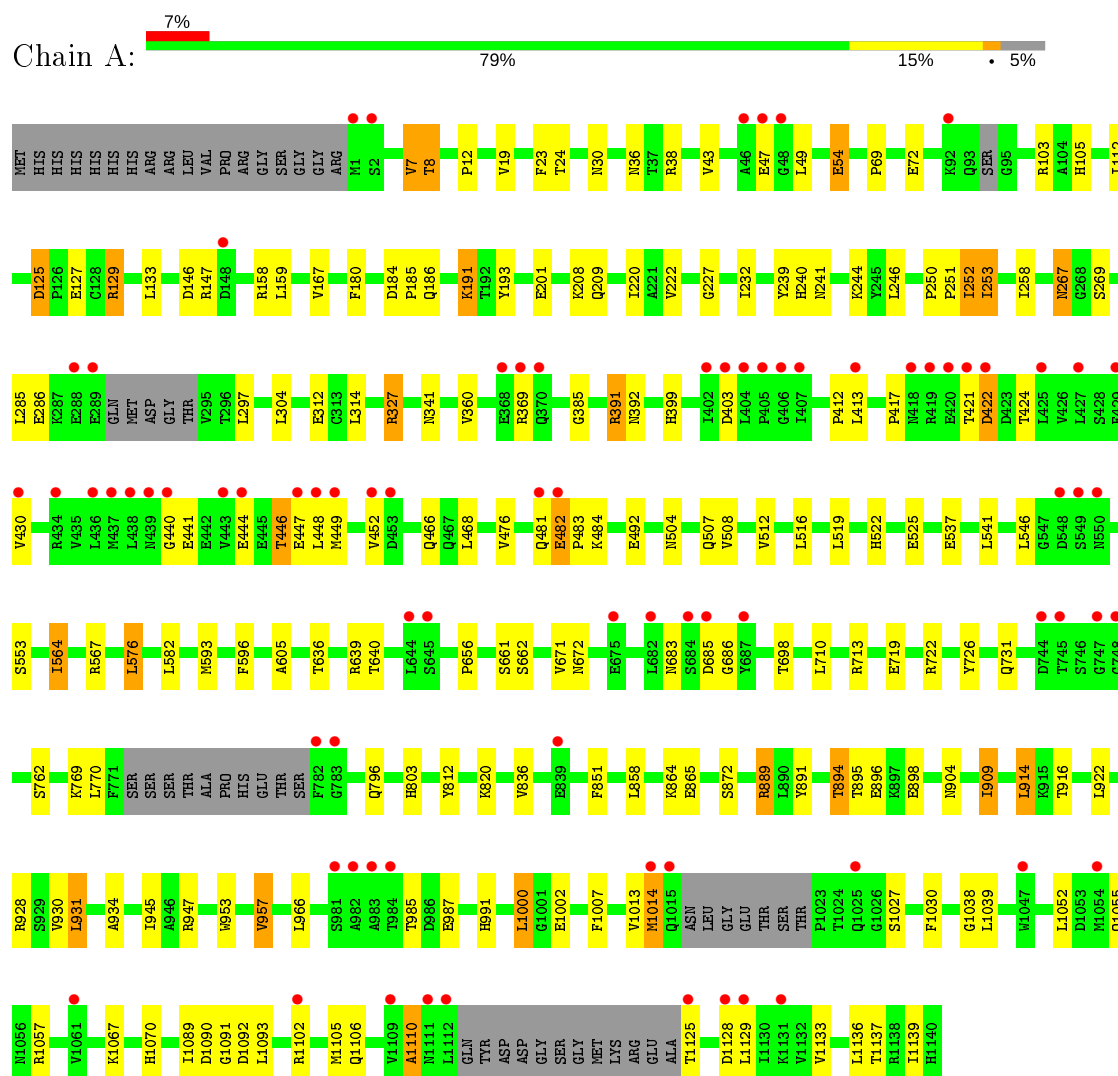
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	479	Total 479	O 479	0	0
4	B	218	Total 218	O 218	0	0

3 Residue-property plots [i](#)

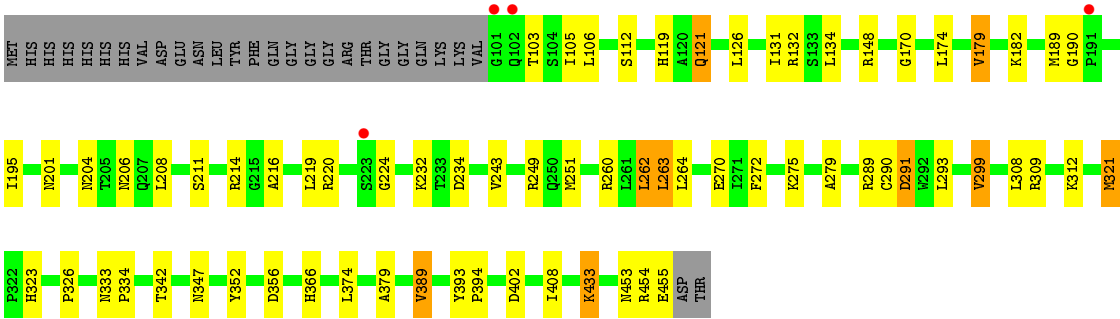
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DNA damage-binding protein 1



• Molecule 2: DNA damage-binding protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.44Å 114.36Å 173.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 48.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.30) 99.8 (48.65-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.208 , 0.251 0.208 , 0.251	Depositor DCC
R_{free} test set	4861 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12246	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: PG4

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	0.43	1/8854 (0.0%)	0.60	3/11989 (0.0%)
2	B	0.43	0/2917	0.65	1/3962 (0.0%)
All	All	0.43	1/11771 (0.0%)	0.61	4/15951 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	LYS	CG-CD	-5.26	1.34	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	208	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	931	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	685	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	422	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

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	8693	0	8672	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2843	0	2788	42	0
3	A	13	0	18	0	0
4	A	479	0	0	17	0
4	B	218	0	0	3	0
All	All	12246	0	11478	160	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 7.

All (160) 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:698:THR:HA	4:A:1511:HOH:O	1.60	1.01
1:A:482:GLU:HB3	1:A:483:PRO:HD3	1.42	1.00
1:A:482:GLU:HB3	1:A:483:PRO:CD	1.91	0.99
1:A:889:ARG:HH11	1:A:889:ARG:HG3	1.30	0.93
1:A:312:GLU:HG2	1:A:327:ARG:HG2	1.53	0.91
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.15	0.90
2:B:232:LYS:HE3	2:B:234:ASP:H	1.43	0.83
1:A:312:GLU:CG	1:A:327:ARG:HG2	2.11	0.80
1:A:934:ALA:HB2	1:A:945:ILE:HD11	1.63	0.79
2:B:121:GLN:HE21	2:B:121:GLN:H	1.30	0.78
1:A:1055:GLN:NE2	1:A:1090:ASP:H	1.82	0.78
1:A:507:GLN:HE22	1:A:553:SER:H	1.32	0.77
2:B:249:ARG:HE	2:B:291:ASP:HB3	1.51	0.76
1:A:403:ASP:HA	4:A:1511:HOH:O	1.84	0.76
1:A:23:PHE:H	1:A:30:ASN:HD22	1.33	0.74
1:A:112:ILE:HD13	2:B:290:CYS:HB2	1.70	0.73
1:A:889:ARG:HG3	1:A:904:ASN:OD1	1.89	0.72
1:A:125:ASP:OD1	1:A:129:ARG:NH1	2.24	0.71
1:A:894:THR:HG21	4:A:1163:HOH:O	1.89	0.71
1:A:481:GLN:HG2	4:A:1440:HOH:O	1.90	0.70
1:A:23:PHE:H	1:A:30:ASN:ND2	1.89	0.70
1:A:507:GLN:NE2	1:A:553:SER:H	1.92	0.68
1:A:392:ASN:HD22	1:A:710:LEU:HD23	1.62	0.65
2:B:105:ILE:HD12	2:B:126:LEU:HD21	1.78	0.65
1:A:8:THR:HG23	1:A:1092:ASP:OD2	1.96	0.64
1:A:522:HIS:HB2	1:A:525:GLU:HG2	1.79	0.64
1:A:596:PHE:HB3	1:A:661:SER:HB2	1.80	0.64
1:A:889:ARG:NH1	1:A:889:ARG:HG3	2.07	0.63
1:A:504:ASN:HD21	1:A:507:GLN:HE21	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:HD2	4:A:1515:HOH:O	1.99	0.61
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.83	0.60
1:A:922:LEU:HD23	1:A:957:VAL:HG13	1.82	0.60
2:B:179:VAL:HG22	2:B:182:LYS:HB2	1.84	0.60
1:A:285:LEU:HB3	1:A:297:LEU:HD11	1.82	0.60
1:A:770:LEU:HD13	1:A:865:GLU:HB2	1.83	0.59
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.83	0.59
2:B:121:GLN:NE2	2:B:121:GLN:H	2.00	0.58
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.84	0.58
1:A:889:ARG:NH1	1:A:904:ASN:OD1	2.36	0.58
1:A:492:GLU:HG3	1:A:512:VAL:HG11	1.85	0.58
1:A:341:ASN:HB2	4:A:1252:HOH:O	2.03	0.58
1:A:916:THR:CG2	4:A:1527:HOH:O	2.51	0.57
1:A:916:THR:HG22	4:A:1527:HOH:O	2.05	0.57
2:B:321:MET:HG2	2:B:352:TYR:CE2	2.40	0.57
2:B:121:GLN:N	2:B:121:GLN:HE21	2.00	0.56
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	1.87	0.56
2:B:105:ILE:CD1	2:B:126:LEU:HD21	2.35	0.56
1:A:947:ARG:NH2	4:A:1420:HOH:O	2.39	0.56
1:A:640:THR:HG22	4:A:1145:HOH:O	2.06	0.55
1:A:421:THR:HB	1:A:683:ASN:O	2.05	0.55
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.37	0.55
1:A:220:ILE:HD11	1:A:232:ILE:HD11	1.89	0.55
1:A:413:LEU:HB3	1:A:424:THR:HB	1.88	0.55
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.87	0.55
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.39	0.55
1:A:391:ARG:HH11	1:A:672:ASN:HD22	1.56	0.54
1:A:201:GLU:HG3	4:A:1173:HOH:O	2.07	0.54
2:B:201:ASN:HB3	2:B:204:ASN:O	2.07	0.54
2:B:394:PRO:HB3	2:B:402:ASP:HB3	1.89	0.54
2:B:263:LEU:HB2	2:B:272:PHE:HB3	1.90	0.53
2:B:121:GLN:HG2	4:B:589:HOH:O	2.08	0.53
1:A:412:PRO:HB2	1:A:422:ASP:OD2	2.09	0.53
2:B:347:ASN:HA	2:B:366:HIS:O	2.08	0.53
1:A:889:ARG:HD2	1:A:891:TYR:CE1	2.43	0.53
1:A:466:GLN:O	1:A:481:GLN:HB2	2.09	0.52
1:A:546:LEU:HD11	1:A:593:MET:HB3	1.92	0.52
1:A:894:THR:CG2	1:A:896:GLU:H	2.22	0.52
1:A:24:THR:H	1:A:30:ASN:HD21	1.59	0.51
1:A:38:ARG:NH1	1:A:54:GLU:OE2	2.40	0.51
2:B:433:LYS:HG2	4:B:579:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:O	1:A:227:GLY:HA2	2.11	0.51
1:A:1125:THR:OG1	1:A:1128:ASP:HB2	2.10	0.50
1:A:522:HIS:HB2	1:A:525:GLU:CG	2.41	0.50
1:A:1013:VAL:CG1	1:A:1014:MET:N	2.75	0.50
1:A:8:THR:HG21	4:A:1391:HOH:O	2.12	0.50
1:A:413:LEU:HD21	1:A:468:LEU:HD21	1.94	0.49
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.30	0.49
1:A:507:GLN:HE22	1:A:553:SER:N	2.05	0.49
2:B:299:VAL:HA	2:B:326:PRO:HB3	1.94	0.49
1:A:722:ARG:NH1	1:A:812[B]:TYR:OH	2.45	0.48
2:B:216:ALA:HB2	2:B:232:LYS:HD2	1.95	0.48
1:A:392:ASN:ND2	1:A:710:LEU:HD23	2.27	0.48
1:A:953:TRP:CD2	2:B:119:HIS:HE1	2.31	0.48
1:A:12:PRO:HG3	1:A:1002:GLU:OE2	2.14	0.48
1:A:239:TYR:HB3	1:A:246:LEU:HB2	1.96	0.47
2:B:389:VAL:HG13	2:B:408:ILE:HG13	1.95	0.47
2:B:262:LEU:HD13	2:B:264:LEU:HD11	1.96	0.47
1:A:836:VAL:HG22	2:B:106:LEU:HD12	1.97	0.47
2:B:220:ARG:NH1	2:B:224:GLY:O	2.47	0.47
1:A:504:ASN:HD21	1:A:507:GLN:NE2	2.13	0.47
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.80	0.46
1:A:312:GLU:HG3	1:A:327:ARG:HG2	1.93	0.46
2:B:232:LYS:HE3	2:B:234:ASP:N	2.21	0.46
2:B:251:MET:CE	2:B:263:LEU:HG	2.45	0.46
1:A:240:HIS:HE1	4:A:1356:HOH:O	1.99	0.46
1:A:481:GLN:O	1:A:482:GLU:HB2	2.15	0.46
1:A:1013:VAL:HG12	1:A:1014:MET:N	2.30	0.46
1:A:417:PRO:HG3	1:A:481:GLN:HB3	1.97	0.45
1:A:987:GLU:O	1:A:991:HIS:HD2	1.99	0.45
1:A:253:ILE:HG13	1:A:258:ILE:HD11	1.99	0.45
1:A:516:LEU:HD11	1:A:541:LEU:HD21	1.98	0.45
1:A:894:THR:HG22	1:A:896:GLU:N	2.32	0.45
1:A:1070:HIS:HE1	1:A:1090:ASP:OD2	2.00	0.45
1:A:851:PHE:HB3	1:A:858:LEU:HD22	1.98	0.45
2:B:232:LYS:HA	2:B:232:LYS:HD2	1.86	0.45
1:A:24:THR:H	1:A:30:ASN:ND2	2.15	0.45
1:A:576:LEU:HG	4:A:1372:HOH:O	2.15	0.44
1:A:953:TRP:CE2	2:B:119:HIS:HE1	2.35	0.44
1:A:158:ARG:HE	2:B:356:ASP:CG	2.20	0.44
1:A:391:ARG:HD3	1:A:672:ASN:ND2	2.32	0.44
1:A:72:GLU:CD	1:A:103:ARG:HH22	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:SER:HA	2:B:216:ALA:O	2.17	0.44
2:B:379:ALA:HA	2:B:389:VAL:O	2.18	0.44
1:A:1102:ARG:HA	1:A:1105:MET:HB2	1.99	0.44
1:A:1027:SER:OG	1:A:1039:LEU:HD11	2.17	0.44
1:A:252:ILE:H	1:A:252:ILE:HG13	1.43	0.44
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.99	0.43
1:A:448:LEU:HD11	1:A:484:LYS:HE2	1.99	0.43
1:A:731:GLN:HA	1:A:796:GLN:NE2	2.33	0.43
1:A:191:LYS:HE3	1:A:193:TYR:CZ	2.53	0.43
2:B:454:ARG:O	2:B:455:GLU:C	2.57	0.43
2:B:170:GLY:C	2:B:195:ILE:HD11	2.38	0.43
2:B:249:ARG:HG2	2:B:251:MET:SD	2.59	0.43
2:B:131:ILE:O	2:B:134:LEU:HB2	2.19	0.43
2:B:275:LYS:NZ	4:B:605:HOH:O	2.41	0.43
1:A:267:ASN:ND2	1:A:269:SER:OG	2.52	0.42
1:A:286:GLU:HG2	4:A:1171:HOH:O	2.18	0.42
1:A:127:GLU:HB2	1:A:129:ARG:NH1	2.34	0.42
1:A:909:ILE:HD13	1:A:928:ARG:HG3	2.01	0.42
1:A:1057:ARG:HH12	1:A:1110:ALA:HB3	1.85	0.42
1:A:19:VAL:HG21	4:A:1292:HOH:O	2.19	0.42
1:A:112:ILE:HD11	2:B:289:ARG:HB2	2.00	0.42
1:A:105:HIS:CE1	1:A:1067:LYS:HD2	2.54	0.42
2:B:323:HIS:HE1	2:B:342:THR:OG1	2.03	0.42
1:A:605:ALA:HB1	1:A:636:THR:HB	2.02	0.42
1:A:446:THR:HG22	1:A:447:GLU:H	1.85	0.42
1:A:449:MET:HB2	1:A:484:LYS:HB3	2.02	0.42
1:A:8:THR:CG2	1:A:1092:ASP:OD2	2.64	0.41
1:A:146:ASP:HB3	4:A:1337:HOH:O	2.20	0.41
1:A:508:VAL:HB	1:A:519:LEU:HB2	2.02	0.41
1:A:894:THR:HG22	1:A:896:GLU:H	1.84	0.41
1:A:185:PRO:HB2	1:A:186:GLN:NE2	2.35	0.41
2:B:333:ASN:HA	2:B:334:PRO:HD3	1.92	0.41
2:B:433:LYS:HD2	2:B:433:LYS:HA	1.90	0.41
1:A:440:GLY:O	1:A:686:GLY:HA3	2.19	0.41
1:A:1007:PHE:CD2	1:A:1030:PHE:HB3	2.56	0.41
2:B:251:MET:HB2	2:B:264:LEU:O	2.21	0.41
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.56	0.40
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.21	0.40
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.95	0.40
1:A:385:GLY:HA3	1:A:719:GLU:O	2.21	0.40
1:A:72:GLU:OE2	1:A:103:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:LEU:CD2	1:A:957:VAL:HG13	2.49	0.40
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.22	0.40
2:B:279:ALA:HB1	2:B:299:VAL:HG22	2.02	0.40
1:A:872:SER:HB3	1:A:914:LEU:HD22	2.03	0.40
1:A:895:THR:OG1	1:A:896:GLU:OE2	2.39	0.40
2:B:299:VAL:HB	2:B:326:PRO:HB3	2.03	0.40
1:A:564:ILE:HG22	1:A:582:LEU:HB2	2.04	0.40
1:A:762:SER:O	1:A:803:HIS:HA	2.22	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	1097/1158 (95%)	1045 (95%)	46 (4%)	6 (0%)	29	35
2	B	353/383 (92%)	331 (94%)	20 (6%)	2 (1%)	25	31
All	All	1450/1541 (94%)	1376 (95%)	66 (5%)	8 (1%)	25	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	GLU
1	A	369	ARG
1	A	1110	ALA
1	A	36	ASN
2	B	291	ASP
1	A	430	VAL
2	B	190	GLY
1	A	564	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	973/1014 (96%)	918 (94%)	55 (6%)	20	28
2	B	313/336 (93%)	286 (91%)	27 (9%)	10	12
All	All	1286/1350 (95%)	1204 (94%)	82 (6%)	17	23

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	8	THR
1	A	43	VAL
1	A	47	GLU
1	A	49	LEU
1	A	54	GLU
1	A	125	ASP
1	A	129	ARG
1	A	133	LEU
1	A	147	ARG
1	A	159	LEU
1	A	191	LYS
1	A	209	GLN
1	A	241	ASN
1	A	244	LYS
1	A	252	ILE
1	A	253	ILE
1	A	267	ASN
1	A	304	LEU
1	A	314	LEU
1	A	327	ARG
1	A	360	VAL
1	A	391	ARG
1	A	399	HIS
1	A	441	GLU
1	A	444	GLU
1	A	446	THR

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Mol	Chain	Res	Type
1	A	452	VAL
1	A	476	VAL
1	A	537	GLU
1	A	567	ARG
1	A	576	LEU
1	A	639	ARG
1	A	662	SER
1	A	713	ARG
1	A	769	LYS
1	A	820	LYS
1	A	864	LYS
1	A	889	ARG
1	A	894	THR
1	A	898	GLU
1	A	909	ILE
1	A	914	LEU
1	A	930	VAL
1	A	931	LEU
1	A	957	VAL
1	A	966	LEU
1	A	985	THR
1	A	1000	LEU
1	A	1014	MET
1	A	1052	LEU
1	A	1089	ILE
1	A	1093	LEU
1	A	1106	GLN
1	A	1129	LEU
2	B	103	THR
2	B	112	SER
2	B	121	GLN
2	B	132	ARG
2	B	148	ARG
2	B	174	LEU
2	B	179	VAL
2	B	189	MET
2	B	206	ASN
2	B	214	ARG
2	B	219	LEU
2	B	243	VAL
2	B	260	ARG
2	B	262	LEU

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Mol	Chain	Res	Type
2	B	263	LEU
2	B	270	GLU
2	B	293	LEU
2	B	299	VAL
2	B	308	LEU
2	B	309	ARG
2	B	312	LYS
2	B	321	MET
2	B	374	LEU
2	B	389	VAL
2	B	393	TYR
2	B	433	LYS
2	B	453	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	30	ASN
1	A	85	ASN
1	A	105	HIS
1	A	186	GLN
1	A	241	ASN
1	A	267	ASN
1	A	374	GLN
1	A	392	ASN
1	A	455	GLN
1	A	465	HIS
1	A	497	ASN
1	A	507	GLN
1	A	648	ASN
1	A	672	ASN
1	A	711	HIS
1	A	727	GLN
1	A	796	GLN
1	A	809	GLN
1	A	852	GLN
1	A	908	ASN
1	A	991	HIS
1	A	1034	ASN
1	A	1055	GLN
1	A	1056	ASN

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Mol	Chain	Res	Type
1	A	1070	HIS
2	B	107	HIS
2	B	116	GLN
2	B	119	HIS
2	B	121	GLN
2	B	124	GLN
2	B	323	HIS
2	B	370	GLN
2	B	419	GLN
2	B	448	ASN
2	B	453	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PG4	A	1141	-	12,12,12	0.49	0	11,11,11	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	A	1141	-	-	4/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1141	PG4	O3-C5-C6-O4
3	A	1141	PG4	O4-C7-C8-O5
3	A	1141	PG4	C4-C3-O2-C2
3	A	1141	PG4	C8-C7-O4-C6

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	1105/1158 (95%)	0.21	78 (7%) 16 21	16, 36, 63, 79	6 (0%)
2	B	355/383 (92%)	-0.11	4 (1%) 80 85	15, 29, 45, 50	4 (1%)
All	All	1460/1541 (94%)	0.13	82 (5%) 24 30	15, 34, 60, 79	10 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	101	GLY	5.9
1	A	404	LEU	5.8
1	A	747	GLY	4.9
1	A	984	THR	4.9
1	A	982	ALA	4.8
1	A	548	ASP	4.8
1	A	406	GLY	4.4
1	A	685	ASP	4.3
1	A	682	LEU	4.3
1	A	407	ILE	4.2
1	A	782	PHE	4.2
1	A	745	THR	4.2
1	A	443	VAL	4.1
1	A	448	LEU	4.0
1	A	369	ARG	4.0
1	A	439	ASN	4.0
1	A	438	LEU	3.8
1	A	449	MET	3.7
1	A	1112	LEU	3.7
2	B	102	GLN	3.6
1	A	1125	THR	3.6
1	A	422	ASP	3.6
1	A	436	LEU	3.6
1	A	403	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	370	GLN	3.5
1	A	748	GLY	3.5
1	A	1129	LEU	3.4
1	A	684	SER	3.4
1	A	418	ASN	3.4
1	A	419	ARG	3.3
1	A	1015	GLN	3.3
1	A	437	MET	3.3
1	A	413	LEU	3.2
1	A	402	ILE	3.0
1	A	1131	LYS	3.0
1	A	48	GLY	3.0
1	A	644	LEU	2.9
1	A	675	GLU	2.8
1	A	983	ALA	2.8
1	A	444	GLU	2.8
1	A	1025	GLN	2.8
1	A	2	SER	2.8
1	A	481	GLN	2.8
1	A	46	ALA	2.7
1	A	447	GLU	2.8
1	A	427	LEU	2.7
1	A	425	LEU	2.7
1	A	405	PRO	2.7
2	B	191	PRO	2.7
1	A	429	PHE	2.7
1	A	1111	ASN	2.6
1	A	420	GLU	2.6
1	A	440	GLY	2.6
1	A	452	VAL	2.6
1	A	1047	TRP	2.6
1	A	783	GLY	2.6
1	A	1	MET	2.5
1	A	687	TYR	2.5
1	A	1102	ARG	2.4
1	A	645	SER	2.4
1	A	434	ARG	2.4
1	A	981	SER	2.4
1	A	549	SER	2.4
1	A	744	ASP	2.3
1	A	368	GLU	2.3
1	A	47	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	288	GLU	2.3
1	A	421	THR	2.3
1	A	289	GLU	2.3
1	A	1061	VAL	2.2
1	A	1128	ASP	2.2
1	A	1109	VAL	2.2
1	A	839	GLU	2.2
1	A	482	GLU	2.1
1	A	92	LYS	2.1
2	B	223	SER	2.1
1	A	430	VAL	2.1
1	A	1014	MET	2.1
1	A	1054	MET	2.1
1	A	550	ASN	2.0
1	A	148	ASP	2.0
1	A	453	ASP	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. 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(\AA^2)	Q<0.9
3	PG4	A	1141	13/13	0.89	0.17	49,51,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.