W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2016 – 05:04 PM EDT

PDB ID	:	5GS2
Title	:	Crystal structure of diabody complex with repebody and MBP
Authors	:	Kim, J.H.; Song, D.H.; Youn, S.J.; Kim, J.W.; Cho, G.; Lee, H.; Lee, J.O.
Deposited on	:	2016-08-13
Resolution	:	3.59 Å(reported)

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

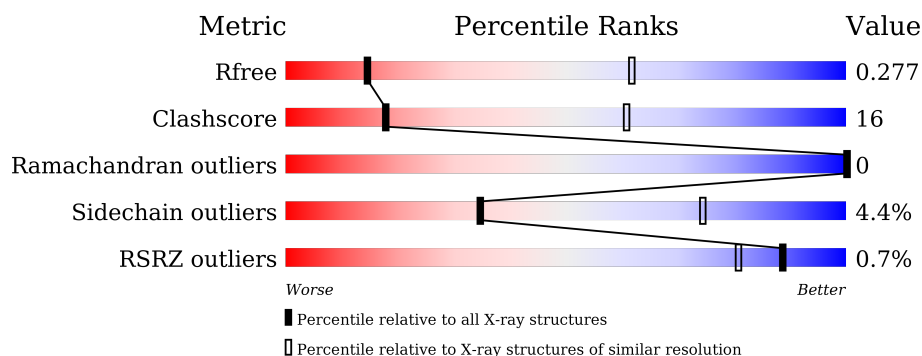|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	Percentile Ranks	Value
Rfree		0.277
Clashscore		16
Ramachandran outliers		0
Sidechain outliers		4.4%
RSRZ outliers		0.7%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 <=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	367	76% 23% •
2	D	233	64% 28% • • •
3	H	239	67% 21% 7% • •
4	B	273	2% 70% 26% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8503 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	4	0
			2874	1855	466	547	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	ASN	ARG	engineered mutation	UNP P0AEX9

• Molecule 2 is a protein called anti-repebody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	226	Total	C	N	O	S	0	2	0
			1733	1091	283	352	7			

• Molecule 3 is a protein called anti-MBP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	231	Total	C	N	O	S	0	4	0
			1791	1130	304	349	8			

• Molecule 4 is a protein called repebody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	268	Total	C	N	O	S	0	0	0
			2105	1336	354	411	4			

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.
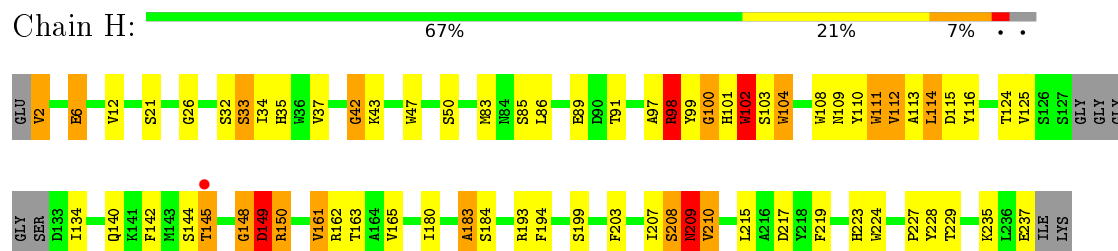
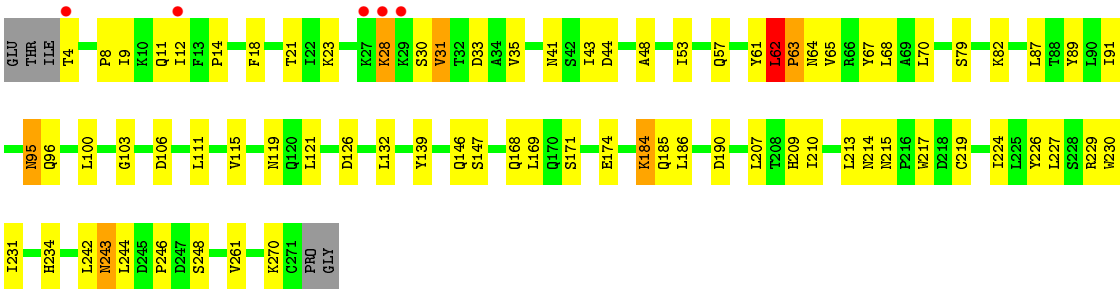- Molecule 1: Maltose-binding periplasmic protein

Chain A:
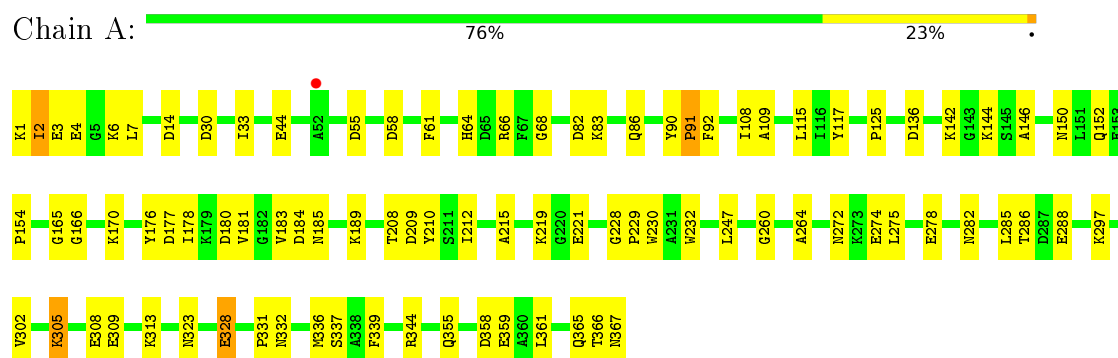
- Molecule 2: anti-repebody

Chain D:
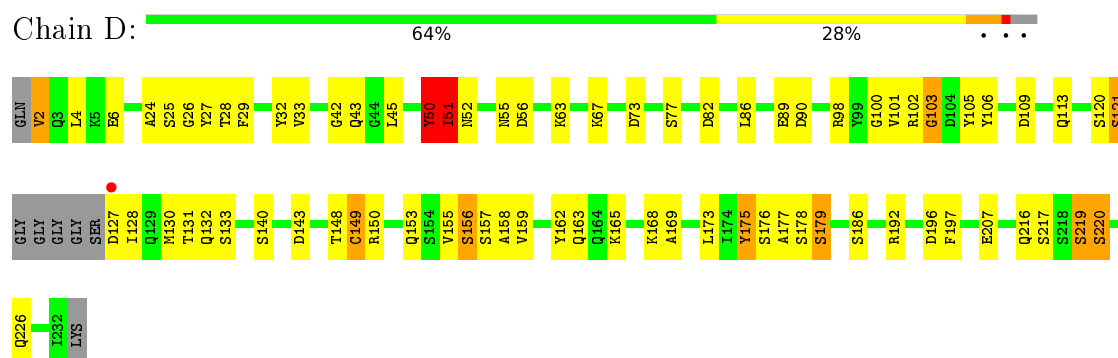
- Molecule 3: anti-MBP

Chain H:

- Molecule 4: repebody

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	278.83Å　　278.83Å　　132.32Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	44.11　–　3.59	Depositor
	44.11　–　3.59	EDS
% Data completeness	99.5 (44.11-3.59)	Depositor
(in resolution range)	96.5 (44.11-3.59)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.01 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.217　,　0.278	Depositor
	0.218　,　0.277	DCC
R_{free} test set	1932 reflections (8.71%)	DCC
Wilson B-factor (Å^2)	88.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.2	EDS
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8503	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ 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)

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	0.54	0/2955	0.69	2/4007 (0.0%)
2	D	0.62	0/1778	0.91	9/2409 (0.4%)
3	H	0.69	1/1851 (0.1%)	1.08	21/2518 (0.8%)
4	B	0.66	4/2143 (0.2%)	0.81	6/2921 (0.2%)
All	All	0.62	5/8727 (0.1%)	0.86	38/11855 (0.3%)

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
3	H	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	243	ASN	N-CA	12.05	1.70	1.46
4	B	244	LEU	N-CA	6.68	1.59	1.46
3	H	102	TRP	CB-CG	-6.46	1.38	1.50
4	B	63	PRO	N-CD	6.17	1.56	1.47
4	B	246	PRO	N-CD	5.28	1.55	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	209	ASN	N-CA-C	-13.80	73.75	111.00
2	D	50	TYR	N-CA-C	-10.41	82.89	111.00
3	H	150	ARG	N-CA-CB	-9.43	93.63	110.60
3	H	208	SER	N-CA-C	9.32	136.18	111.00
3	H	209	ASN	CB-CA-C	9.21	128.82	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	184	SER	N-CA-C	8.77	134.67	111.00
4	B	243	ASN	CB-CA-C	8.47	127.33	110.40
1	A	92	PHE	N-CA-CB	-8.36	95.56	110.60
3	H	100	GLY	N-CA-C	-7.74	93.74	113.10
3	H	148	GLY	N-CA-C	-7.74	93.76	113.10
3	H	149	ASP	CB-CA-C	-7.35	95.71	110.40
3	H	42	GLY	N-CA-C	7.29	131.32	113.10
3	H	111	TRP	N-CA-C	7.26	130.61	111.00
2	D	103	GLY	N-CA-C	-7.07	95.42	113.10
3	H	110	TYR	CB-CA-C	6.66	123.72	110.40
3	H	102	TRP	N-CA-CB	-6.62	98.67	110.60
3	H	183	ALA	N-CA-C	-6.59	93.21	111.00
3	H	210	VAL	N-CA-C	-6.57	93.27	111.00
4	B	62	LEU	N-CA-C	-6.53	93.37	111.00
2	D	42	GLY	N-CA-C	6.50	129.36	113.10
2	D	177	ALA	CB-CA-C	-6.39	100.52	110.10
3	H	150	ARG	N-CA-C	6.38	128.23	111.00
3	H	101	HIS	N-CA-C	6.31	128.05	111.00
1	A	91	PRO	CB-CA-C	-6.27	96.33	112.00
4	B	126	ASP	N-CA-C	-6.19	94.28	111.00
4	B	62	LEU	C-N-CD	-6.17	107.02	120.60
3	H	98	ARG	NE-CZ-NH1	-6.09	117.25	120.30
3	H	101	HIS	N-CA-CB	-6.06	99.69	110.60
2	D	219	SER	N-CA-CB	-5.81	101.79	110.50
4	B	234	HIS	N-CA-CB	-5.75	100.25	110.60
2	D	51	ILE	N-CA-CB	-5.66	97.78	110.80
3	H	208	SER	CB-CA-C	-5.62	99.43	110.10
2	D	43	GLN	N-CA-CB	5.35	120.24	110.60
3	H	113	ALA	N-CA-C	-5.31	96.67	111.00
2	D	179	SER	N-CA-C	5.07	124.68	111.00
2	D	178	SER	N-CA-CB	5.06	118.09	110.50
3	H	215	LEU	CA-CB-CG	5.02	126.86	115.30
4	B	95	ASN	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	220	SER	Peptide
3	H	104	TRP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2874	0	2871	61	0
2	D	1733	0	1677	68	0
3	H	1791	0	1697	89	3
4	B	2105	0	2123	62	3
All	All	8503	0	8368	266	3

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 16.

All (266) 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)
4:B:243:ASN:CA	4:B:243:ASN:N	1.70	1.50
3:H:149:ASP:O	3:H:208:SER:O	1.53	1.27
3:H:99:TYR:CD1	3:H:112:VAL:HG12	1.70	1.24
3:H:149:ASP:CB	3:H:210:VAL:CG2	2.22	1.18
3:H:149:ASP:HB2	3:H:210:VAL:CB	1.74	1.17
3:H:149:ASP:HB3	3:H:210:VAL:HG23	1.27	1.12
3:H:149:ASP:CB	3:H:210:VAL:HG23	1.84	1.06
3:H:149:ASP:HB2	3:H:210:VAL:HB	1.30	1.05
2:D:175:TYR:CE1	2:D:179:SER:OG	2.08	1.04
3:H:149:ASP:CB	3:H:210:VAL:HB	1.86	1.03
3:H:149:ASP:CB	3:H:210:VAL:CB	2.36	1.02
3:H:149:ASP:HB3	3:H:210:VAL:CG2	1.88	1.00
3:H:149:ASP:OD2	3:H:210:VAL:CB	2.10	1.00
3:H:115:ASP:OD1	3:H:116:TYR:CD1	2.16	0.98
3:H:115:ASP:OD1	3:H:116:TYR:N	2.02	0.92
3:H:99:TYR:CD2	3:H:100:GLY:O	2.22	0.92
3:H:115:ASP:OD1	3:H:116:TYR:CG	2.23	0.92
4:B:41:ASN:O	4:B:64:ASN:ND2	2.02	0.91
2:D:103:GLY:HA2	4:B:171:SER:HB2	1.51	0.90
3:H:193:ARG:HD2	3:H:209:ASN:O	1.71	0.90
3:H:149:ASP:CG	3:H:210:VAL:HB	1.91	0.89
2:D:175:TYR:CD1	2:D:179:SER:OG	2.22	0.89
3:H:149:ASP:OD2	3:H:210:VAL:HG11	1.70	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:ASN:O	2:D:56:ASP:CG	2.11	0.88
4:B:61:TYR:C	4:B:62:LEU:HD23	1.95	0.86
2:D:165:LYS:NZ	2:D:207:GLU:O	2.09	0.85
2:D:162:TYR:OH	3:H:114:LEU:HD12	1.77	0.85
3:H:149:ASP:OD2	3:H:210:VAL:CG1	2.24	0.84
3:H:42:GLY:O	3:H:43:LYS:HD3	1.78	0.82
3:H:149:ASP:OD2	3:H:210:VAL:HG21	1.80	0.81
3:H:148:GLY:HA2	3:H:209:ASN:OD1	1.82	0.79
3:H:149:ASP:OD2	3:H:210:VAL:HB	1.80	0.79
3:H:149:ASP:OD2	3:H:210:VAL:CG2	2.31	0.79
4:B:43:ILE:HD12	4:B:62:LEU:HD13	1.65	0.77
3:H:99:TYR:CG	3:H:112:VAL:HG12	2.20	0.77
1:A:166:GLY:HA2	1:A:185:ASN:HD21	1.49	0.76
3:H:149:ASP:CG	3:H:210:VAL:CB	2.54	0.75
4:B:61:TYR:O	4:B:62:LEU:HD23	1.87	0.74
4:B:243:ASN:CB	4:B:243:ASN:N	2.52	0.72
1:A:189[B]:LYS:NZ	1:A:358:ASP:OD1	2.22	0.72
2:D:175:TYR:HE1	2:D:179:SER:CB	2.03	0.72
3:H:103:SER:O	3:H:104:TRP:HB3	1.90	0.71
3:H:149:ASP:HB2	3:H:210:VAL:N	2.06	0.71
3:H:149:ASP:CG	3:H:210:VAL:CG2	2.59	0.70
3:H:91:THR:HG23	3:H:124:THR:HA	1.73	0.70
3:H:99:TYR:CD1	3:H:112:VAL:CG1	2.64	0.69
1:A:4:GLU:HA	1:A:272:ASN:HD21	1.56	0.69
4:B:115:VAL:HG22	4:B:139:TYR:HD2	1.57	0.69
4:B:243:ASN:C	4:B:243:ASN:N	2.44	0.68
2:D:101:VAL:HA	2:D:105:TYR:O	1.94	0.68
1:A:108:ILE:HD13	1:A:285:LEU:HD21	1.75	0.67
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.77	0.67
2:D:105:TYR:OH	2:D:109:ASP:OD1	2.08	0.67
4:B:43:ILE:HD12	4:B:62:LEU:CD1	2.26	0.66
2:D:140:SER:OG	2:D:143:ASP:OD2	2.11	0.66
2:D:89:GLU:N	2:D:89:GLU:OE1	2.27	0.65
3:H:149:ASP:HB2	3:H:210:VAL:CG2	2.04	0.65
3:H:149:ASP:CG	3:H:210:VAL:HG21	2.18	0.64
1:A:184:ASP:HB3	1:A:365:GLN:NE2	2.13	0.64
1:A:1:LYS:NZ	1:A:2:ILE:O	2.31	0.64
4:B:185:GLN:HG2	4:B:209:HIS:HB2	1.79	0.64
1:A:91:PRO:HG2	2:D:219:SER:HB3	1.80	0.64
2:D:52:ASN:O	2:D:56:ASP:OD1	2.16	0.64
3:H:149:ASP:C	3:H:150:ARG:HG3	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:99:TYR:CE1	3:H:112:VAL:HA	2.33	0.63
2:D:120:SER:OG	2:D:121:SER:N	2.30	0.62
2:D:175:TYR:HE1	2:D:179:SER:HB2	1.64	0.62
2:D:175:TYR:CE1	2:D:179:SER:CB	2.79	0.62
1:A:90:TYR:OH	1:A:308:GLU:HG2	2.00	0.62
2:D:67:LYS:NZ	2:D:90:ASP:OD2	2.33	0.62
2:D:55:ASN:HB2	2:D:56:ASP:HA	1.81	0.62
3:H:102:TRP:HZ3	3:H:111:TRP:HB2	1.62	0.62
1:A:165:GLY:O	1:A:185:ASN:ND2	2.33	0.62
3:H:32:SER:HA	3:H:100:GLY:HA2	1.82	0.62
3:H:99:TYR:CE2	3:H:100:GLY:O	2.53	0.61
2:D:51:ILE:HG12	2:D:56:ASP:OD2	2.01	0.61
4:B:213:LEU:HB3	4:B:248:SER:HB2	1.82	0.60
3:H:149:ASP:CB	3:H:210:VAL:HG21	2.29	0.60
4:B:23:LYS:HD2	4:B:30:SER:O	2.01	0.60
1:A:365:GLN:C	1:A:367:ASN:H	2.04	0.60
4:B:242:LEU:HD23	4:B:243:ASN:HB2	1.84	0.60
2:D:63:LYS:NZ	3:H:89:GLU:OE1	2.35	0.59
1:A:355:GLN:HB3	1:A:359:GLU:HB2	1.83	0.59
3:H:144:SER:HA	3:H:237:GLU:HB2	1.85	0.59
3:H:149:ASP:HB2	3:H:210:VAL:CA	2.31	0.59
1:A:64:HIS:HE1	1:A:260:GLY:HA2	1.66	0.59
1:A:64:HIS:CE1	1:A:260:GLY:HA2	2.37	0.59
1:A:152:GLN:HG2	1:A:209:ASP:HB3	1.85	0.59
3:H:102:TRP:CZ3	3:H:111:TRP:HB2	2.37	0.59
4:B:30:SER:OG	4:B:31:VAL:N	2.36	0.58
4:B:62:LEU:N	4:B:63:PRO:CD	2.66	0.58
3:H:42:GLY:C	3:H:43:LYS:HD3	2.22	0.58
2:D:6:GLU:O	2:D:113:GLN:NE2	2.36	0.58
1:A:150:ASN:ND2	1:A:210:TYR:HB2	2.19	0.58
1:A:68:GLY:HA3	1:A:332:ASN:O	2.03	0.57
4:B:61:TYR:O	4:B:62:LEU:CD2	2.52	0.57
3:H:161:VAL:HG23	3:H:224:TRP:HB2	1.87	0.57
1:A:309:GLU:OE1	2:D:192:ARG:NH2	2.37	0.57
4:B:115:VAL:HG22	4:B:139:TYR:CD2	2.40	0.57
1:A:4:GLU:HA	1:A:272:ASN:ND2	2.18	0.57
2:D:163:GLN:NE2	2:D:165:LYS:HD3	2.20	0.57
4:B:9:ILE:HD12	4:B:28:LYS:HZ3	1.69	0.57
2:D:217:SER:OG	3:H:111:TRP:HA	2.04	0.56
1:A:142:LYS:HB2	1:A:144:LYS:HG2	1.87	0.56
2:D:32:TYR:HD1	2:D:100:GLY:HA2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:LYS:HB2	1:A:55:ASP:HB3	1.87	0.56
4:B:215:ASN:HB2	4:B:217:TRP:NE1	2.21	0.56
3:H:140:GLN:HG3	3:H:142:PHE:O	2.06	0.56
2:D:33:VAL:HG11	2:D:50:TYR:CD2	2.41	0.56
2:D:150:ARG:NH2	2:D:196:ASP:OD2	2.38	0.56
1:A:181:VAL:HG12	1:A:183:VAL:HG22	1.88	0.55
3:H:35:HIS:CE1	3:H:50[A]:SER:HG	2.24	0.55
1:A:150:ASN:HD22	1:A:210:TYR:HB2	1.72	0.55
2:D:131:THR:O	2:D:149:CYS:HA	2.06	0.55
2:D:128:ILE:HG21	2:D:216:GLN:HG3	1.90	0.54
1:A:282:ASN:O	1:A:286:THR:HG21	2.07	0.54
4:B:230:TRP:HE3	4:B:231:ILE:HD13	1.73	0.54
2:D:132:GLN:HG2	2:D:149:CYS:HB2	1.89	0.54
1:A:184:ASP:HB3	1:A:365:GLN:CD	2.28	0.54
4:B:219:CYS:HA	4:B:224:ILE:HG21	1.89	0.54
3:H:162:ARG:O	3:H:163:THR:HG22	2.08	0.54
3:H:99:TYR:CG	3:H:100:GLY:O	2.60	0.54
1:A:82:ASP:O	1:A:86:GLN:HG3	2.07	0.53
2:D:52:ASN:N	2:D:56:ASP:OD1	2.42	0.53
4:B:23:LYS:HD3	4:B:31:VAL:HG12	1.89	0.53
2:D:32:TYR:CD1	2:D:100:GLY:HA2	2.44	0.53
4:B:62:LEU:HD23	4:B:62:LEU:N	2.22	0.53
2:D:157:SER:OG	2:D:192:ARG:NH1	2.39	0.53
4:B:67:TYR:HD1	4:B:89:TYR:HB2	1.73	0.52
3:H:6:GLU:HA	3:H:21:SER:O	2.09	0.52
2:D:168:LYS:HD2	2:D:169:ALA:H	1.73	0.52
1:A:361:LEU:O	1:A:365:GLN:NE2	2.43	0.51
4:B:95:ASN:O	4:B:119:ASN:OD1	2.28	0.51
1:A:7:LEU:HA	1:A:58:ASP:OD2	2.10	0.51
2:D:33:VAL:HG22	2:D:52:ASN:HB2	1.92	0.51
3:H:149:ASP:HB2	3:H:210:VAL:HG23	1.74	0.51
1:A:328:GLU:OE1	3:H:102:TRP:HA	2.10	0.51
3:H:34:ILE:HD13	3:H:98:ARG:HA	1.92	0.51
3:H:97:ALA:HB1	3:H:114:LEU:HB3	1.93	0.51
3:H:35:HIS:HD1	3:H:50[B]:SER:HG	0.61	0.50
1:A:90:TYR:CD1	1:A:305:LYS:HG3	2.47	0.50
2:D:101:VAL:HB	2:D:106:TYR:CE1	2.47	0.50
1:A:183:VAL:HG23	1:A:365:GLN:HG3	1.93	0.50
2:D:103:GLY:HA2	4:B:171:SER:CB	2.34	0.50
1:A:288:GLU:H	1:A:288:GLU:CD	2.15	0.49
3:H:149:ASP:HB2	3:H:210:VAL:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:CE1	1:A:305:LYS:HG3	2.47	0.49
2:D:220:SER:OG	3:H:109:ASN:ND2	2.45	0.49
1:A:247:LEU:HD12	1:A:323:ASN:HD21	1.76	0.49
2:D:127:ASP:CG	2:D:128:ILE:H	2.16	0.49
3:H:199:SER:HA	3:H:203:PHE:HE1	1.78	0.49
4:B:62:LEU:N	4:B:63:PRO:HD3	2.27	0.49
2:D:155:VAL:HG23	2:D:156:SER:O	2.12	0.49
1:A:219:LYS:HZ2	1:A:221:GLU:CD	2.16	0.49
4:B:111:LEU:HD12	4:B:132:LEU:HD22	1.93	0.49
2:D:155:VAL:HG11	2:D:216:GLN:HG3	1.95	0.49
1:A:136:ASP:HA	1:A:146:ALA:HB2	1.94	0.49
2:D:51:ILE:HG23	2:D:51:ILE:O	2.13	0.49
3:H:98:ARG:O	3:H:98:ARG:HG2	2.13	0.49
1:A:228:GLY:HA3	1:A:230:TRP:CH2	2.48	0.48
4:B:186:LEU:O	4:B:210:ILE:HA	2.14	0.48
4:B:227:LEU:O	4:B:231:ILE:HG12	2.12	0.48
4:B:8:PRO:HA	4:B:33:ASP:O	2.13	0.48
3:H:227:PRO:O	3:H:229:THR:HG23	2.13	0.48
1:A:177:ASP:OD2	1:A:180:ASP:HB2	2.12	0.48
4:B:48:ALA:HB3	4:B:70:LEU:HD23	1.94	0.48
2:D:29:PHE:CD2	2:D:77:SER:HA	2.49	0.48
2:D:163:GLN:HB2	2:D:173:LEU:HD11	1.95	0.47
2:D:157:SER:N	2:D:192:ARG:NH1	2.62	0.47
1:A:176:TYR:CE2	1:A:331:PRO:HB3	2.49	0.47
1:A:66:ARG:NH1	1:A:337:SER:HA	2.29	0.47
2:D:216:GLN:OE1	2:D:216:GLN:O	2.32	0.47
3:H:149:ASP:H	3:H:210:VAL:H	1.63	0.47
1:A:66:ARG:HH12	1:A:337:SER:HA	1.79	0.47
4:B:9:ILE:HA	4:B:12:ILE:HD12	1.96	0.47
3:H:162:ARG:O	3:H:163:THR:CG2	2.63	0.47
4:B:226:TYR:HA	4:B:229:ARG:HD3	1.96	0.46
2:D:192:ARG:HD2	2:D:197:PHE:CE2	2.50	0.46
4:B:67:TYR:CD1	4:B:89:TYR:HB2	2.50	0.46
2:D:127:ASP:CG	2:D:128:ILE:N	2.69	0.46
2:D:2:VAL:HA	2:D:25:SER:O	2.15	0.46
2:D:2:VAL:HA	2:D:26:GLY:HA3	1.97	0.46
1:A:44:GLU:HB2	1:A:66:ARG:HD2	1.98	0.46
4:B:9:ILE:HD12	4:B:28:LYS:NZ	2.30	0.46
2:D:132:GLN:H	2:D:226:GLN:HE22	1.62	0.46
1:A:1:LYS:HG3	1:A:2:ILE:N	2.31	0.46
4:B:4:THR:O	4:B:4:THR:OG1	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:TYR:O	2:D:175:TYR:CD1	2.69	0.45
4:B:79:SER:HB3	4:B:82:LYS:NZ	2.31	0.45
4:B:9:ILE:HG12	4:B:35:VAL:HG11	1.97	0.45
4:B:100:LEU:HD23	4:B:100:LEU:HA	1.70	0.45
1:A:212:ILE:HA	1:A:215:ALA:HB3	1.98	0.45
2:D:101:VAL:HB	2:D:106:TYR:HE1	1.81	0.45
3:H:148:GLY:HA2	3:H:209:ASN:CG	2.36	0.45
4:B:18:PHE:HD1	4:B:53:ILE:HD13	1.82	0.45
4:B:43:ILE:CD1	4:B:62:LEU:CD1	2.95	0.45
1:A:33:ILE:HG12	1:A:275:LEU:HD13	1.98	0.45
4:B:184:LYS:HA	4:B:207:LEU:HA	1.98	0.44
4:B:190:ASP:OD1	4:B:214:ASN:ND2	2.48	0.44
4:B:103:GLY:HA2	4:B:106:ASP:OD1	2.17	0.44
3:H:194:PHE:CD1	3:H:207:ILE:HG12	2.53	0.44
1:A:208:THR:HG23	1:A:212:ILE:HG23	1.99	0.44
2:D:130:MET:SD	2:D:216:GLN:HB2	2.58	0.44
2:D:98:ARG:HH21	2:D:109:ASP:CG	2.21	0.44
3:H:102:TRP:HZ3	3:H:111:TRP:CB	2.30	0.44
1:A:154:PRO:HD3	1:A:344:ARG:HB3	1.99	0.44
1:A:170:LYS:HB2	1:A:180:ASP:OD1	2.18	0.44
3:H:98:ARG:NH1	3:H:100:GLY:HA3	2.32	0.44
4:B:215:ASN:HB2	4:B:217:TRP:CE2	2.52	0.43
4:B:14:PRO:HD2	4:B:57:GLN:O	2.19	0.43
3:H:33:SER:HG	3:H:99:TYR:HD2	1.65	0.43
4:B:242:LEU:C	4:B:243:ASN:CA	2.71	0.43
3:H:12:VAL:O	3:H:125:VAL:HA	2.18	0.43
1:A:30:ASP:OD1	1:A:30:ASP:N	2.52	0.43
4:B:121:LEU:HD23	4:B:121:LEU:HA	1.79	0.43
3:H:35:HIS:NE2	3:H:99:TYR:HB2	2.33	0.43
1:A:189[B]:LYS:NZ	1:A:358:ASP:CG	2.72	0.43
4:B:146:GLN:O	4:B:169:LEU:HA	2.18	0.43
4:B:219:CYS:HB3	4:B:261:VAL:HG21	2.01	0.43
3:H:2:VAL:HA	3:H:26:GLY:HA3	2.01	0.43
2:D:133:SER:HB2	2:D:148:THR:OG1	2.18	0.43
2:D:4:LEU:HD23	2:D:24:ALA:HA	2.01	0.42
3:H:165:VAL:HG11	3:H:203:PHE:CD1	2.55	0.42
4:B:91:ILE:HG23	4:B:115:VAL:HB	2.01	0.42
2:D:45:LEU:HD11	3:H:219:PHE:CZ	2.54	0.42
3:H:217:ASP:HB2	3:H:235:LYS:HG3	2.01	0.42
3:H:83:MET:HB3	3:H:86:LEU:HD21	2.02	0.42
3:H:99:TYR:C	3:H:100:GLY:O	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLU:O	1:A:278:GLU:HG3	2.19	0.42
2:D:106:TYR:HE2	4:B:147:SER:HB3	1.85	0.42
2:D:162:TYR:CZ	3:H:114:LEU:HD12	2.52	0.42
3:H:33:SER:OG	3:H:99:TYR:HD2	2.02	0.42
3:H:223:HIS:HB2	3:H:228:TYR:CZ	2.54	0.42
3:H:115:ASP:CG	3:H:116:TYR:N	2.70	0.42
1:A:365:GLN:C	1:A:367:ASN:N	2.72	0.42
1:A:90:TYR:HA	1:A:91:PRO:HD3	1.92	0.42
4:B:65:VAL:HG11	4:B:68:LEU:HB2	2.02	0.42
2:D:159:VAL:HG21	2:D:197:PHE:CD1	2.55	0.42
2:D:33:VAL:HG11	2:D:50:TYR:HD2	1.84	0.42
3:H:145:THR:HG21	3:H:210:VAL:HG21	2.01	0.42
1:A:14:ASP:O	1:A:297:LYS:HD3	2.20	0.42
3:H:103:SER:HA	3:H:108:TRP:HA	2.00	0.41
1:A:109:ALA:CB	1:A:302:VAL:HA	2.50	0.41
3:H:199:SER:HA	3:H:203:PHE:CE1	2.55	0.41
1:A:55:ASP:N	1:A:55:ASP:OD1	2.54	0.41
4:B:44:ASP:N	4:B:44:ASP:OD1	2.44	0.41
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.55	0.41
1:A:183:VAL:O	1:A:361:LEU:HB3	2.20	0.41
2:D:175:TYR:HD1	2:D:175:TYR:O	2.04	0.41
3:H:180:ILE:CG2	3:H:183:ALA:O	2.68	0.41
1:A:336:MET:HA	1:A:339:PHE:HB3	2.02	0.41
2:D:156:SER:O	2:D:158:ALA:N	2.54	0.41
2:D:176:SER:O	2:D:176:SER:OG	2.28	0.41
4:B:23:LYS:O	4:B:23:LYS:HG3	2.20	0.40
2:D:128:ILE:CD1	2:D:153:GLN:HB2	2.51	0.40
3:H:99:TYR:HE1	3:H:112:VAL:HA	1.81	0.40
1:A:117:TYR:CE2	1:A:125:PRO:HD3	2.57	0.40
4:B:146:GLN:HG2	4:B:168:GLN:HB2	2.03	0.40
3:H:207:ILE:CG2	3:H:210:VAL:HG22	2.51	0.40
1:A:61:PHE:CE2	1:A:264:ALA:HB2	2.57	0.40
2:D:27:TYR:HB2	4:B:270:LYS:HE2	2.03	0.40
2:D:28:THR:HG23	4:B:270:LYS:HE3	2.03	0.40
1:A:115:LEU:HB2	1:A:247:LEU:HD23	2.04	0.40
4:B:21:THR:HG21	4:B:48:ALA:HB2	2.03	0.40
4:B:87:LEU:HD12	4:B:87:LEU:HA	1.96	0.40
3:H:102:TRP:HZ3	3:H:111:TRP:CG	2.40	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:150:ARG:CD	4:B:64:ASN:OD1[8_555]	1.68	0.52
3:H:150:ARG:CG	4:B:64:ASN:OD1[8_555]	1.92	0.28
3:H:150:ARG:CB	4:B:64:ASN:OD1[8_555]	1.94	0.26

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	369/367 (100%)	349 (95%)	20 (5%)	0	100	100
2	D	224/233 (96%)	204 (91%)	20 (9%)	0	100	100
3	H	231/239 (97%)	213 (92%)	18 (8%)	0	100	100
4	B	266/273 (97%)	242 (91%)	24 (9%)	0	100	100
All	All	1090/1112 (98%)	1008 (92%)	82 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	298/294 (101%)	289 (97%)	9 (3%)	48	82
2	D	195/196 (100%)	183 (94%)	12 (6%)	23	65
3	H	194/194 (100%)	181 (93%)	13 (7%)	20	62
4	B	245/249 (98%)	238 (97%)	7 (3%)	50	82
All	All	932/933 (100%)	891 (96%)	41 (4%)	35	74

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All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	GLU
1	A	6	LYS
1	A	83	LYS
1	A	178	ILE
1	A	305	LYS
1	A	313	LYS
1	A	328	GLU
1	A	366	THR
2	D	2	VAL
2	D	50	TYR
2	D	51	ILE
2	D	73	ASP
2	D	82	ASP
2	D	86	LEU
2	D	102	ARG
2	D	121	SER
2	D	149	CYS
2	D	156	SER
2	D	175	TYR
2	D	186	SER
3	H	2	VAL
3	H	6	GLU
3	H	33	SER
3	H	85	SER
3	H	98	ARG
3	H	102	TRP
3	H	112	VAL
3	H	114	LEU
3	H	134	ILE
3	H	145	THR
3	H	149	ASP
3	H	161	VAL
3	H	209	ASN
4	B	11	GLN
4	B	28	LYS
4	B	31	VAL
4	B	62	LEU
4	B	96	GLN
4	B	174	GLU
4	B	184	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	164	GLN
4	B	64	ASN
4	B	119	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 (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	367/367 (100%)	-0.14	1 (0%)	94	90	58, 93, 140, 166	0
2	D	226/233 (96%)	-0.21	1 (0%)	93	88	58, 82, 119, 133	0
3	H	231/239 (96%)	-0.23	1 (0%)	93	88	57, 81, 125, 153	0
4	B	268/273 (98%)	0.02	5 (1%)	70	56	59, 93, 140, 183	0
All	All	1092/1112 (98%)	-0.13	8 (0%)	89	81	57, 87, 135, 183	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	4	THR	6.5
4	B	29	LYS	3.6
1	A	52	ALA	3.2
4	B	28	LYS	2.4
4	B	27	LYS	2.3
3	H	145	THR	2.1
4	B	12	ILE	2.1
2	D	127	ASP	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.