



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:39 AM UTC

PDB ID : 4CEH / pdb_00004ceh
Title : Crystal structure of AddAB with a forked DNA substrate
Authors : Krajewski, W.W.; Wilkinson, M.; Fu, X.; Cronin, N.B.; Wigley, D.
Deposited on : 2013-11-11
Resolution : 3.24 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

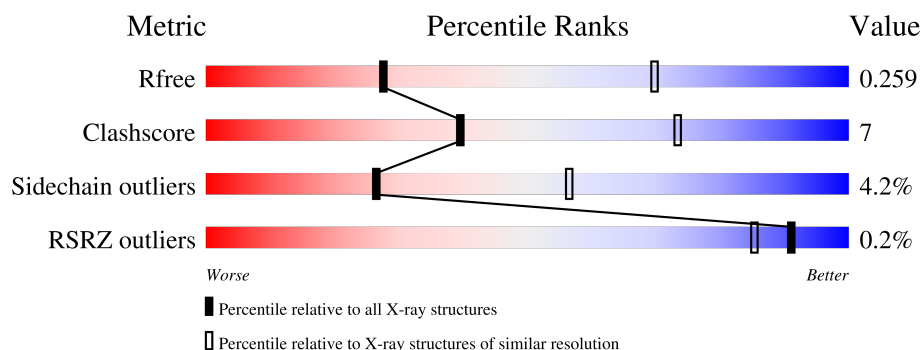
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	1232	 76% 17% 6%
2	B	1166	 78% 20% ..
3	X	65	 31% 26% 43%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19433 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 ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1154	Total	C	N	O	S	0	0	0
			9339	5966	1589	1757	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	GLY	ALA	variant	UNP P23478
A	1172	ALA	ASP	engineered mutation	UNP P23478

- Molecule 2 is a protein called ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1148	Total	C	N	O	S	0	0	0
			9330	5929	1597	1760	44			

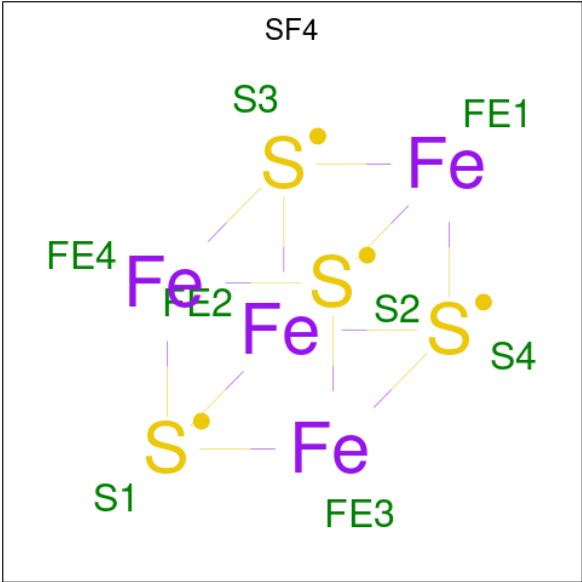
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	843	ASP	GLU	variant	UNP P23477
B	844	GLU	GLN	variant	UNP P23477
B	961	ALA	ASP	engineered mutation	UNP P23477

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	37	Total	C	N	O	P	0	0	0
			756	363	126	230	37			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

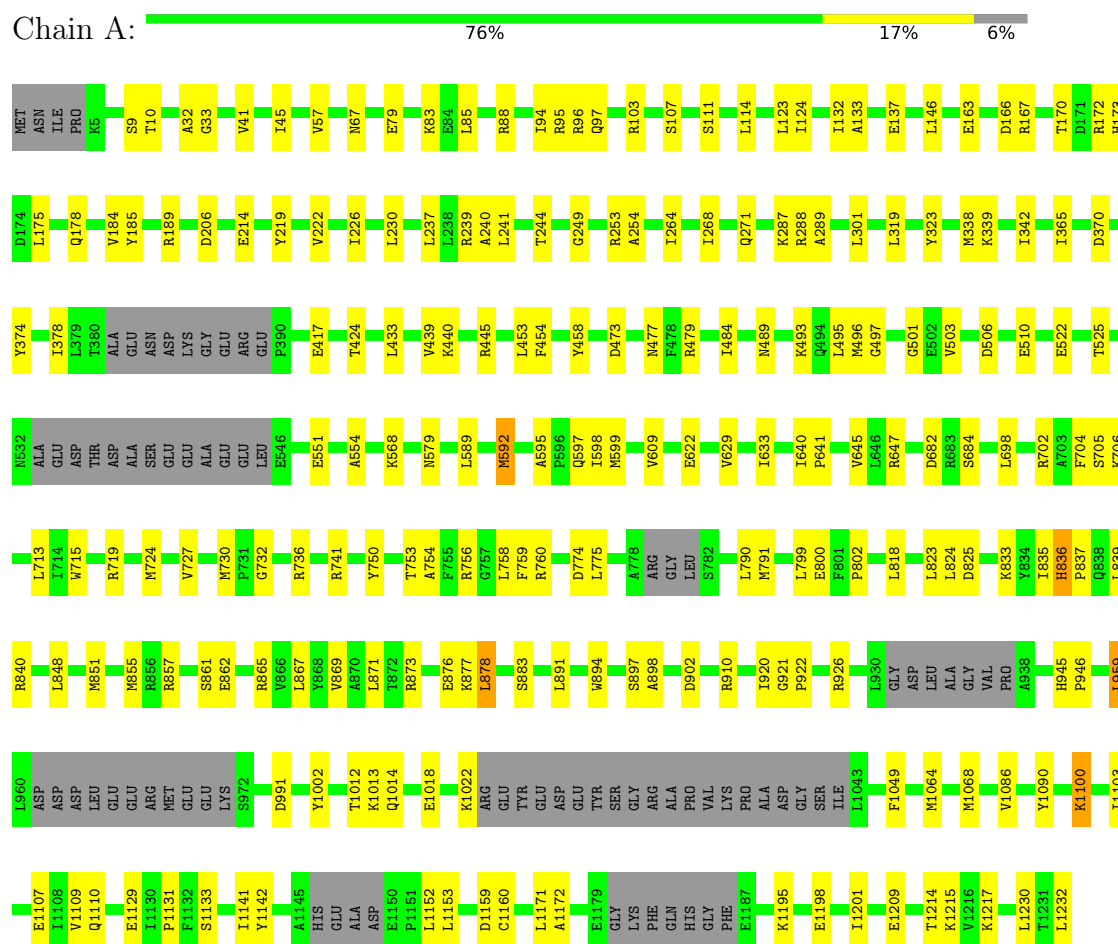


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		

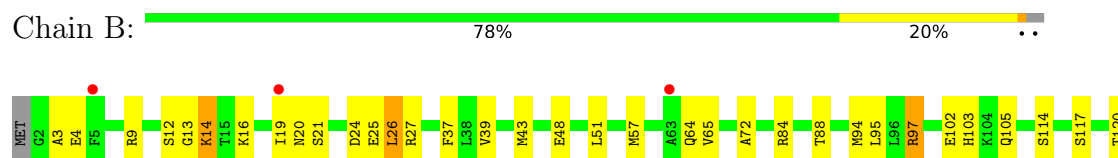
3 Residue-property plots [i](#)

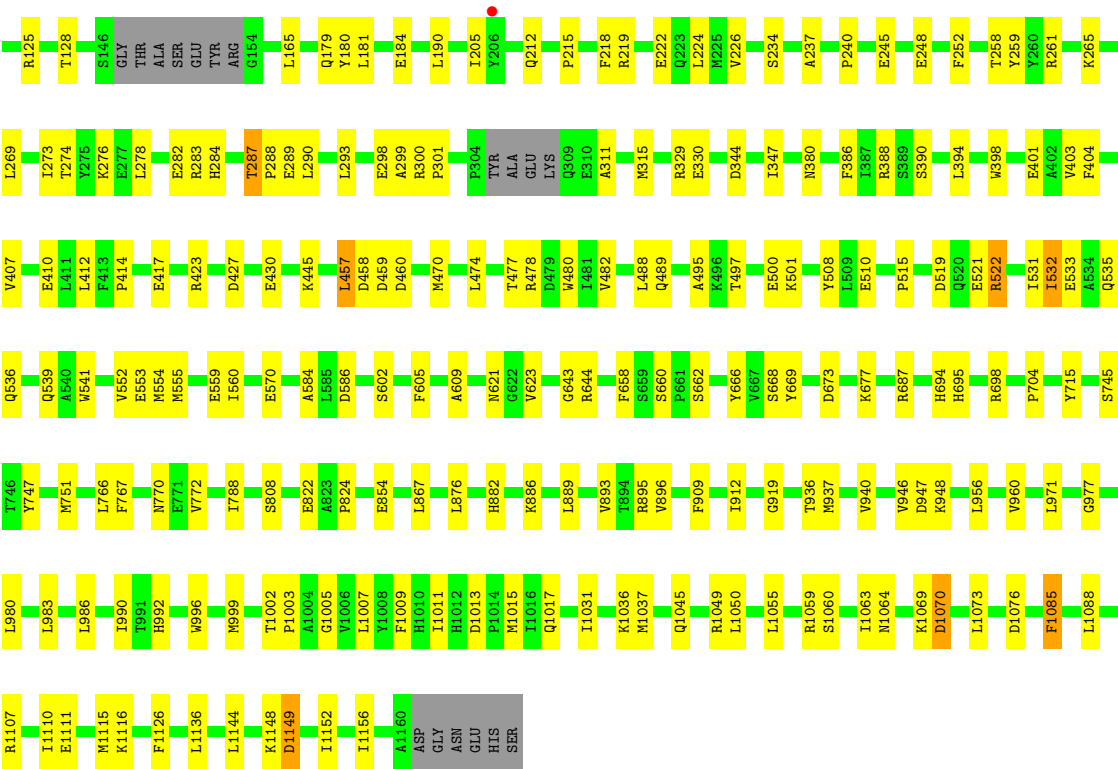
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ATP-DEPENDENT HELICASE/NUCLEASE SUBUNIT A

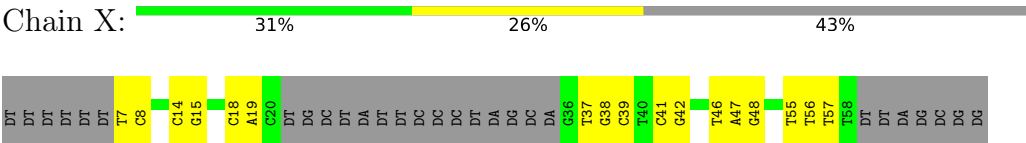


• Molecule 2: ATP-DEPENDENT HELICASE/DEOXYRIBONUCLEASE SUBUNIT B





● Molecule 3: DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.37Å 96.77Å 109.69Å 104.38° 96.11° 90.03°	Depositor
Resolution (Å)	29.94 – 3.24 29.94 – 3.24	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.94-3.24) 97.8 (29.94-3.24)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.229 , 0.264 (Not available) , 0.259	Depositor DCC
R_{free} test set	2376 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	96.4	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19433	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: SF4

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	0.27	0/9524	0.73	6/12849 (0.0%)
2	B	0.26	0/9518	0.72	6/12824 (0.0%)
3	X	0.24	0/843	0.48	0/1297
All	All	0.26	0/19885	0.71	12/26970 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	287	THR	CA-C-N	6.66	126.45	119.05
2	B	287	THR	C-N-CA	6.66	126.45	119.05
1	A	592	MET	CA-C-N	-6.49	112.94	119.56
1	A	592	MET	C-N-CA	-6.49	112.94	119.56
1	A	1142	TYR	CA-C-N	5.62	124.81	118.97
1	A	1142	TYR	C-N-CA	5.62	124.81	118.97
1	A	836	HIS	CA-C-N	5.44	125.09	119.05
1	A	836	HIS	C-N-CA	5.44	125.09	119.05
2	B	660	SER	CA-C-N	-5.43	113.99	120.13
2	B	660	SER	C-N-CA	-5.43	113.99	120.13
2	B	621	ASN	N-CA-C	5.17	117.59	110.35
2	B	482	VAL	CB-CA-C	-5.12	107.30	114.00

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	9339	0	9335	131	0
2	B	9330	0	9280	132	0
3	X	756	0	424	13	0
4	B	8	0	0	0	0
All	All	19433	0	19039	257	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 (257) 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)
2:B:284:HIS:HB3	2:B:290:LEU:HB3	1.64	0.76
1:A:287:LYS:NZ	3:X:19:DA:OP1	2.20	0.75
1:A:825:ASP:HB2	1:A:851:MET:HE3	1.69	0.74
2:B:896:VAL:HG21	2:B:1011:ILE:HG23	1.73	0.71
1:A:1090:TYR:HB2	1:A:1100:LYS:HG3	1.73	0.70
1:A:167:ARG:NH1	1:A:835:ILE:O	2.24	0.69
1:A:88:ARG:HD2	1:A:94:ILE:HG13	1.73	0.69
1:A:1013:LYS:NZ	2:B:48:GLU:OE1	2.28	0.66
2:B:245:GLU:OE2	2:B:261:ARG:NH2	2.28	0.65
1:A:79:GLU:OE2	1:A:83:LYS:NZ	2.30	0.65
2:B:1070:ASP:OD1	2:B:1070:ASP:N	2.22	0.65
2:B:445:LYS:O	2:B:478:ARG:NH2	2.29	0.65
1:A:836:HIS:HD2	1:A:839:LEU:H	1.45	0.64
1:A:170:THR:HG23	1:A:172:ARG:H	1.62	0.64
2:B:788:ILE:HB	2:B:937:MET:HG2	1.79	0.64
1:A:96:ARG:HD2	2:B:644:ARG:HH22	1.62	0.64
2:B:300:ARG:H	2:B:300:ARG:HD3	1.63	0.64
2:B:212:GLN:HA	2:B:258:THR:HG21	1.78	0.64
2:B:414:PRO:HB2	2:B:417:GLU:HG3	1.81	0.63
2:B:165:LEU:HD11	2:B:623:VAL:HG11	1.78	0.63
2:B:97:ARG:NH2	2:B:114:SER:O	2.32	0.62
2:B:386:PHE:HE1	2:B:412:LEU:HG	1.65	0.62
2:B:909:PHE:HB3	2:B:947:ASP:HB3	1.81	0.62
2:B:4:GLU:HG3	2:B:274:THR:HB	1.82	0.61
2:B:289:GLU:OE1	2:B:695:HIS:NE2	2.27	0.61
2:B:248:GLU:OE1	2:B:644:ARG:NH1	2.33	0.61
1:A:163:GLU:OE1	1:A:167:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1045:GLN:HE21	2:B:1049:ARG:HD2	1.66	0.61
1:A:622:GLU:OE2	1:A:736:ARG:NH1	2.34	0.60
1:A:715:TRP:CD1	1:A:719:ARG:HH21	2.19	0.60
1:A:253:ARG:HE	1:A:289:ALA:HB1	1.66	0.60
1:A:554:ALA:HB2	1:A:959:LEU:HD21	1.83	0.59
2:B:300:ARG:HG2	2:B:301:PRO:HD3	1.83	0.59
2:B:497:THR:HA	2:B:559:GLU:HA	1.84	0.58
2:B:1149:ASP:OD1	2:B:1149:ASP:N	2.37	0.58
2:B:410:GLU:OE2	2:B:423:ARG:NH1	2.34	0.58
2:B:13:GLY:N	2:B:282:GLU:OE1	2.35	0.58
1:A:682:ASP:OD2	1:A:684:SER:OG	2.20	0.57
1:A:898:ALA:HB1	1:A:926:ARG:HG3	1.86	0.57
2:B:12:SER:O	2:B:14:LYS:N	2.37	0.57
1:A:123:LEU:HD12	1:A:378:ILE:HG23	1.86	0.57
1:A:867:LEU:HD21	1:A:920:ILE:HD11	1.85	0.57
1:A:1160:CYS:HB3	1:A:1171:LEU:HB3	1.85	0.57
1:A:484:ILE:HD12	1:A:878:LEU:HD13	1.86	0.56
2:B:4:GLU:OE2	2:B:276:LYS:NZ	2.32	0.56
1:A:114:LEU:HD13	1:A:132:ILE:HD11	1.86	0.56
2:B:990:ILE:HG13	2:B:1003:PRO:HG3	1.87	0.56
2:B:205:ILE:HD13	2:B:224:LEU:HD13	1.86	0.56
1:A:1133:SER:HB3	1:A:1153:LEU:HD11	1.86	0.56
1:A:704:PHE:HD2	1:A:713:LEU:HD23	1.71	0.56
1:A:759:PHE:HE2	2:B:401:GLU:HG3	1.71	0.56
1:A:1209:GLU:HG2	1:A:1215:LYS:HA	1.88	0.56
1:A:724:MET:HE1	1:A:741:ARG:HG3	1.87	0.55
1:A:424:THR:HG21	1:A:433:LEU:HB2	1.88	0.55
2:B:180:TYR:OH	2:B:553:GLU:OE1	2.24	0.55
2:B:919:GLY:HA3	2:B:940:VAL:HG12	1.89	0.55
2:B:1036:LYS:HE3	2:B:1064:ASN:HA	1.89	0.55
2:B:26:LEU:HB3	2:B:57:MET:HE1	1.89	0.54
2:B:912:ILE:HD11	2:B:948:LYS:HB3	1.89	0.54
2:B:16:LYS:NZ	2:B:20:ASN:OD1	2.34	0.54
2:B:1059:ARG:NH2	2:B:1076:ASP:OD2	2.38	0.54
1:A:702:ARG:NH2	2:B:427:ASP:OD2	2.41	0.54
2:B:14:LYS:NZ	2:B:234:SER:OG	2.38	0.54
2:B:673:ASP:OD1	2:B:677:LYS:N	2.38	0.54
1:A:85:LEU:HD11	1:A:95:ARG:HG2	1.90	0.53
1:A:137:GLU:CD	1:A:753:THR:HG23	2.33	0.53
1:A:833:LYS:NZ	2:B:1017:GLN:OE1	2.41	0.53
1:A:754:ALA:O	1:A:760:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:977:GLY:HA2	2:B:980:LEU:HD21	1.90	0.53
3:X:47:DA:H4'	3:X:48:DG:OP1	2.08	0.53
2:B:609:ALA:HB3	2:B:669:TYR:HB3	1.89	0.53
1:A:705:SER:HB2	1:A:758:LEU:HD13	1.90	0.53
1:A:146:LEU:HD13	1:A:178:GLN:HB2	1.92	0.52
2:B:72:ALA:HA	2:B:190:LEU:HD13	1.91	0.52
2:B:240:PRO:HB2	2:B:259:TYR:CD2	2.43	0.52
2:B:19:ILE:HG23	2:B:51:LEU:HD23	1.91	0.52
1:A:184:VAL:HG22	1:A:824:LEU:HD21	1.91	0.52
2:B:956:LEU:HD23	2:B:1002:THR:HB	1.90	0.52
1:A:1215:LYS:HD3	1:A:1217:LYS:HZ2	1.74	0.52
2:B:284:HIS:CD2	2:B:290:LEU:HD12	2.44	0.51
1:A:497:GLY:H	1:A:501:GLY:HA3	1.73	0.51
2:B:24:ASP:OD1	2:B:27:ARG:NH1	2.44	0.50
2:B:983:LEU:HD13	2:B:1088:LEU:HB3	1.92	0.50
3:X:41:DC:H2''	3:X:42:DG:C8	2.46	0.50
1:A:268:ILE:HA	1:A:271:GLN:HG3	1.92	0.50
2:B:1107:ARG:NH2	2:B:1111:GLU:OE1	2.40	0.50
1:A:525:THR:HG23	1:A:878:LEU:HB3	1.93	0.50
2:B:1152:ILE:O	2:B:1156:ILE:HG13	2.12	0.50
1:A:791:MET:HE1	1:A:799:LEU:HD12	1.94	0.50
2:B:386:PHE:CE1	2:B:412:LEU:HG	2.47	0.50
2:B:477:THR:HA	2:B:480:TRP:NE1	2.27	0.50
1:A:439:VAL:HG23	1:A:454:PHE:CD1	2.47	0.49
1:A:869:VAL:O	1:A:873:ARG:HG2	2.11	0.49
2:B:315:MET:HE2	2:B:666:TYR:HB3	1.94	0.49
1:A:185:TYR:O	1:A:189:ARG:HG2	2.12	0.49
1:A:774:ASP:OD1	1:A:775:LEU:N	2.44	0.49
1:A:1214:THR:OG1	1:A:1215:LYS:N	2.35	0.49
1:A:241:LEU:O	1:A:244:THR:OG1	2.28	0.49
2:B:772:VAL:HG21	2:B:1110:ILE:HG13	1.95	0.49
2:B:495:ALA:HB1	2:B:500:GLU:HG3	1.94	0.49
1:A:32:ALA:O	1:A:477:ASN:ND2	2.44	0.49
2:B:222:GLU:O	2:B:226:VAL:HG23	2.12	0.49
1:A:440:LYS:HG2	1:A:496:MET:HE1	1.95	0.49
1:A:1014:GLN:HG3	1:A:1152:LEU:HD13	1.95	0.48
2:B:347:ILE:HG12	2:B:605:PHE:HB2	1.94	0.48
2:B:770:ASN:H	2:B:1136:LEU:HD21	1.77	0.48
2:B:315:MET:HE3	2:B:668:SER:HB3	1.96	0.48
2:B:535:GLN:HG2	2:B:539:GLN:HE21	1.79	0.48
2:B:519:ASP:OD1	2:B:522:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:960:VAL:HG22	2:B:1007:LEU:HB2	1.95	0.48
1:A:756:ARG:H	1:A:756:ARG:HD2	1.78	0.48
2:B:287:THR:HG21	2:B:311:ALA:HB2	1.94	0.48
1:A:818:LEU:HD21	1:A:855:MET:HB3	1.96	0.47
1:A:871:LEU:HG	1:A:878:LEU:HD21	1.96	0.47
2:B:1055:LEU:HD22	2:B:1060:SER:HB2	1.96	0.47
1:A:107:SER:HB3	1:A:111:SER:HB3	1.97	0.47
1:A:589:LEU:HD11	1:A:598:ILE:HD12	1.96	0.47
1:A:1018:GLU:O	1:A:1022:LYS:HG3	2.15	0.47
1:A:1159:ASP:HB2	1:A:1172:ALA:HA	1.97	0.47
1:A:124:ILE:HG13	1:A:374:TYR:HD1	1.80	0.47
1:A:445:ARG:N	1:A:862:GLU:OE2	2.40	0.47
2:B:95:LEU:HB2	2:B:554:MET:HE2	1.96	0.47
2:B:293:LEU:HD21	2:B:658:PHE:HB3	1.95	0.47
2:B:1009:PHE:HD2	2:B:1037:MET:HE2	1.78	0.47
2:B:1115:MET:HB2	2:B:1144:LEU:HB2	1.96	0.47
1:A:522:GLU:O	1:A:877:LYS:NZ	2.40	0.47
1:A:1107:GLU:HA	1:A:1110:GLN:HB2	1.97	0.47
1:A:568:LYS:NZ	1:A:579:ASN:OD1	2.38	0.47
1:A:802:PRO:HB3	1:A:876:GLU:HG3	1.96	0.47
2:B:876:LEU:HA	2:B:882:HIS:HB3	1.96	0.46
1:A:67:ASN:ND2	3:X:57:DT:OP2	2.44	0.46
1:A:206:ASP:OD1	1:A:339:LYS:NZ	2.46	0.46
1:A:991:ASP:HA	2:B:745:SER:HB3	1.96	0.46
1:A:599:MET:HG2	1:A:609:VAL:HG11	1.97	0.46
2:B:488:LEU:HD13	2:B:508:TYR:HB2	1.96	0.46
3:X:46:DT:H2''	3:X:47:DA:C8	2.51	0.46
2:B:971:LEU:HD22	2:B:1149:ASP:HB3	1.98	0.46
1:A:706:LYS:NZ	2:B:521:GLU:OE2	2.46	0.46
1:A:1195:LYS:HA	1:A:1198:GLU:HB2	1.97	0.46
2:B:14:LYS:HG2	2:B:278:LEU:HD12	1.97	0.46
2:B:533:GLU:O	2:B:536:GLN:HG2	2.16	0.46
1:A:249:GLY:HA2	1:A:301:LEU:HD22	1.98	0.45
3:X:7:DT:H2''	3:X:8:DC:C6	2.51	0.45
3:X:55:DT:H1'	3:X:56:DT:H5'	1.98	0.45
1:A:226:ILE:HG12	1:A:319:LEU:HD11	1.96	0.45
1:A:647:ARG:HH21	2:B:772:VAL:HG22	1.81	0.45
2:B:394:LEU:HG	2:B:489:GLN:HG3	1.98	0.45
2:B:532:ILE:HD12	2:B:533:GLU:H	1.81	0.45
1:A:57:VAL:HG23	1:A:97:GLN:OE1	2.16	0.45
2:B:532:ILE:H	2:B:532:ILE:HG13	1.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ASN:O	1:A:493:LYS:HB2	2.17	0.45
1:A:840:ARG:NH2	2:B:1015:MET:HG2	2.32	0.45
2:B:21:SER:O	2:B:25:GLU:HG2	2.17	0.45
2:B:457:LEU:HD12	2:B:867:LEU:HD22	1.99	0.45
1:A:288:ARG:NH2	3:X:39:DC:O2	2.50	0.45
1:A:133:ALA:HB2	1:A:365:ILE:HG23	1.99	0.44
1:A:33:GLY:HA3	1:A:477:ASN:ND2	2.33	0.44
1:A:264:ILE:O	1:A:268:ILE:HG13	2.17	0.44
1:A:551:GLU:OE1	1:A:883:SER:OG	2.34	0.44
1:A:861:SER:O	1:A:865:ARG:HG3	2.18	0.44
2:B:117:SER:O	2:B:120:THR:HG22	2.16	0.44
2:B:404:PHE:CZ	2:B:430:GLU:HA	2.53	0.44
1:A:1002:TYR:OH	2:B:586:ASP:OD2	2.29	0.44
2:B:102:GLU:HG3	2:B:103:HIS:ND1	2.33	0.44
2:B:215:PRO:O	2:B:219:ARG:HG2	2.18	0.44
1:A:214:GLU:HA	1:A:219:TYR:CD2	2.53	0.44
1:A:592:MET:HE1	1:A:791:MET:HA	2.00	0.44
1:A:103:ARG:HH21	2:B:643:GLY:HA3	1.83	0.44
2:B:398:TRP:HE1	2:B:489:GLN:NE2	2.16	0.44
2:B:992:HIS:O	2:B:996:TRP:HB3	2.17	0.44
2:B:283:ARG:HG3	2:B:662:SER:HA	1.99	0.44
2:B:330:GLU:OE2	2:B:698:ARG:NH1	2.50	0.44
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.82	0.43
2:B:299:ALA:O	2:B:687:ARG:NH2	2.43	0.43
1:A:495:LEU:HA	1:A:910:ARG:HD3	1.99	0.43
1:A:1049:PHE:CD1	2:B:552:VAL:HG21	2.53	0.43
2:B:704:PRO:HG3	2:B:715:TYR:CE2	2.53	0.43
2:B:986:LEU:HD21	2:B:1003:PRO:HB3	2.00	0.43
2:B:94:MET:HB3	2:B:555:MET:HE2	2.00	0.43
2:B:747:TYR:O	2:B:751:MET:HG2	2.19	0.43
2:B:822:GLU:HB3	2:B:824:PRO:HD2	2.00	0.43
3:X:47:DA:H1'	3:X:48:DG:O5'	2.18	0.43
1:A:597:GLN:H	1:A:597:GLN:NE2	2.16	0.43
1:A:1086:VAL:HG12	1:A:1100:LYS:HD3	1.99	0.43
2:B:205:ILE:HG21	2:B:224:LEU:HD13	2.01	0.43
2:B:273:ILE:H	2:B:273:ILE:HG13	1.77	0.43
1:A:836:HIS:HA	1:A:837:PRO:HD3	1.81	0.43
1:A:595:ALA:HA	1:A:790:LEU:HD21	2.00	0.43
2:B:39:VAL:HB	2:B:43:MET:HB3	2.01	0.43
2:B:808:SER:HG	2:B:1126:PHE:HE2	1.67	0.43
1:A:41:VAL:O	1:A:45:ILE:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG13	1:A:323:TYR:CE1	2.53	0.42
1:A:1129:GLU:O	1:A:1131:PRO:HD3	2.19	0.42
2:B:895:ARG:NH1	2:B:1031:ILE:HG21	2.35	0.42
1:A:597:GLN:H	1:A:597:GLN:HE21	1.67	0.42
1:A:704:PHE:CD2	1:A:713:LEU:HD23	2.54	0.42
2:B:501:LYS:NZ	2:B:560:ILE:O	2.42	0.42
2:B:912:ILE:HB	2:B:946:VAL:HG23	2.02	0.42
1:A:240:ALA:O	1:A:244:THR:HG23	2.20	0.42
1:A:417:GLU:HG2	1:A:453:LEU:HD11	2.02	0.42
2:B:84:ARG:HD2	2:B:181:LEU:HB2	2.01	0.42
2:B:237:ALA:HA	2:B:252:PHE:CD1	2.54	0.42
2:B:515:PRO:HG3	2:B:541:TRP:CH2	2.55	0.42
3:X:37:DT:H2"	3:X:38:DG:C8	2.55	0.42
1:A:458:TYR:OH	1:A:473:ASP:OD2	2.24	0.42
1:A:732:GLY:O	1:A:736:ARG:HG3	2.19	0.42
2:B:12:SER:HB2	2:B:278:LEU:HB3	2.01	0.42
2:B:37:PHE:HB3	2:B:65:VAL:HA	2.02	0.42
1:A:479:ARG:NE	1:A:800:GLU:OE1	2.45	0.42
1:A:756:ARG:HH11	2:B:380:ASN:ND2	2.17	0.42
1:A:945:HIS:HA	1:A:946:PRO:HD3	1.83	0.42
2:B:128:THR:HG23	2:B:184:GLU:HG3	2.02	0.42
1:A:124:ILE:HD13	1:A:124:ILE:H	1.84	0.42
1:A:823:LEU:HB3	1:A:851:MET:HE2	2.02	0.42
1:A:85:LEU:HD12	1:A:85:LEU:HA	1.77	0.41
1:A:840:ARG:NH2	2:B:1013:ASP:O	2.53	0.41
2:B:403:VAL:O	2:B:407:VAL:HG23	2.19	0.41
1:A:1201:ILE:HG13	1:A:1232:LEU:HD12	2.02	0.41
1:A:370:ASP:HB3	1:A:374:TYR:CD2	2.55	0.41
1:A:1141:ILE:HD12	1:A:1152:LEU:HD11	2.02	0.41
2:B:344:ASP:HB3	2:B:602:SER:HB2	2.03	0.41
1:A:9:SER:O	1:A:10:THR:HG22	2.20	0.41
1:A:338:MET:O	1:A:342:ILE:HG12	2.20	0.41
1:A:501:GLY:C	1:A:503:VAL:H	2.29	0.41
1:A:1012:THR:OG1	2:B:584:ALA:O	2.38	0.41
2:B:9:ARG:HH22	2:B:298:GLU:HG2	1.86	0.41
2:B:105:GLN:H	2:B:105:GLN:CD	2.28	0.41
1:A:230:LEU:HD12	1:A:271:GLN:HE21	1.85	0.41
1:A:244:THR:HG21	1:A:254:ALA:HB2	2.01	0.41
1:A:727:VAL:HA	1:A:730:MET:HG2	2.02	0.41
1:A:170:THR:HG23	1:A:173:HIS:H	1.85	0.41
1:A:506:ASP:O	1:A:510:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ALA:HB3	2:B:273:ILE:HG22	2.03	0.41
2:B:388:ARG:HD2	2:B:570:GLU:CD	2.46	0.41
2:B:470:MET:HE3	2:B:474:LEU:HD21	2.01	0.41
1:A:239:ARG:HD3	1:A:239:ARG:HA	1.85	0.41
1:A:629:VAL:O	1:A:633:ILE:HG13	2.21	0.41
1:A:641:PRO:O	1:A:645:VAL:HG23	2.21	0.41
1:A:698:LEU:O	1:A:702:ARG:HG2	2.21	0.41
1:A:897:SER:HB3	1:A:922:PRO:HB3	2.03	0.41
2:B:226:VAL:HG22	2:B:269:LEU:HD22	2.03	0.41
2:B:386:PHE:O	2:B:390:SER:OG	2.37	0.41
2:B:889:LEU:O	2:B:893:VAL:HG23	2.20	0.41
2:B:971:LEU:HB3	2:B:1152:ILE:HG21	2.02	0.41
2:B:1005:GLY:HA2	2:B:1085:PHE:CZ	2.56	0.41
2:B:1069:LYS:HE3	3:X:15:DG:H3'	2.02	0.41
3:X:18:DC:H2''	3:X:19:DA:C8	2.56	0.41
1:A:175:LEU:O	1:A:178:GLN:HG2	2.20	0.41
2:B:329:ARG:HD3	2:B:715:TYR:HA	2.03	0.41
2:B:287:THR:HA	2:B:288:PRO:HD3	1.74	0.40
1:A:166:ASP:HB3	1:A:837:PRO:HB3	2.03	0.40
1:A:640:ILE:HB	1:A:641:PRO:HD3	2.02	0.40
1:A:750:TYR:OH	1:A:760:ARG:HB3	2.21	0.40
3:X:14:DC:H2''	3:X:15:DG:C8	2.56	0.40
1:A:894:TRP:CE2	1:A:921:GLY:HA3	2.57	0.40
1:A:959:LEU:HD12	1:A:959:LEU:HA	1.89	0.40
2:B:1050:LEU:HD23	2:B:1050:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	354/1062 (33%)	341 (96%)	13 (4%)	30	59
2	B	695/1029 (68%)	664 (96%)	31 (4%)	24	55
All	All	1049/2091 (50%)	1005 (96%)	44 (4%)	26	56

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	LEU
1	A	848	LEU
1	A	857	ARG
1	A	878	LEU
1	A	891	LEU
1	A	902	ASP
1	A	959	LEU
1	A	1064	MET
1	A	1068	MET
1	A	1100	LYS
1	A	1103	ILE
1	A	1109	VAL
1	A	1230	LEU
2	B	14	LYS
2	B	26	LEU
2	B	64	GLN
2	B	88	THR
2	B	97	ARG
2	B	125	ARG
2	B	179	GLN
2	B	218	PHE
2	B	265	LYS
2	B	457	LEU
2	B	458	ASP
2	B	459	ASP
2	B	460	ASP
2	B	510	GLU
2	B	522	ARG
2	B	531	ILE
2	B	532	ILE
2	B	694	HIS
2	B	766	LEU
2	B	767	PHE

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Mol	Chain	Res	Type
2	B	854	GLU
2	B	886	LYS
2	B	936	THR
2	B	999	MET
2	B	1063	ILE
2	B	1070	ASP
2	B	1073	LEU
2	B	1085	PHE
2	B	1116	LYS
2	B	1148	LYS
2	B	1149	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	A	271	GLN
1	A	836	HIS
1	A	912	GLN
1	A	952	GLN
1	A	1004	HIS
2	B	170	GLN
2	B	270	ASN
2	B	316	GLN
2	B	428	GLN
2	B	463	GLN
2	B	489	GLN
2	B	723	GLN
2	B	729	GLN
2	B	817	GLN
2	B	933	ASN
2	B	1045	GLN
2	B	1131	GLN

5.3.3 RNA ⓘ

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](#)

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	$\# Z > 2$
4	SF4	B	2161	2	0,12,12	-	-	-		

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
4	SF4	B	2161	2	-	-	0/6/5/5

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 [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	1154/1232 (93%)	-0.23	0 100 100	64, 115, 170, 194	0
2	B	1148/1166 (98%)	-0.12	4 (0%) 90 81	68, 123, 159, 185	1 (0%)
3	X	37/65 (56%)	0.06	0 100 100	120, 191, 215, 222	0
All	All	2339/2463 (94%)	-0.17	4 (0%) 91 85	64, 121, 168, 222	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	63	ALA	2.2
2	B	19	ILE	2.1
2	B	206	TYR	2.1
2	B	5	PHE	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 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	SF4	B	2161	8/8	0.98	0.05	79,104,112,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.