



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:40 PM UTC

PDB ID : 3AAD / pdb_00003aad
Title : Structure of the histone chaperone CIA/ASF1-double bromodomain complex linking histone modifications and site-specific histone eviction
Authors : Akai, Y.; Adachi, N.; Hayashi, Y.; Eitoku, M.; Sano, N.; Natsume, R.; Kudo, N.; Tanokura, M.; Senda, T.; Horikoshi, M.
Deposited on : 2009-11-16
Resolution : 3.30 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 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

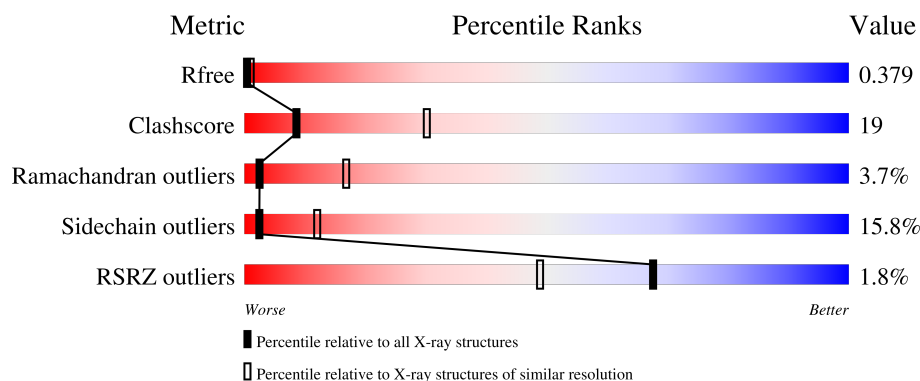
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	292	0.3% 48% 36% 5% 10%
2	B	158	3% 42% 38% 14% . .
2	D	158	2% 59% 29% 7% . .

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	SO4	A	400	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4617 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 Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2164	1369	367	417	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1338	GLY	-	expression tag	UNP P21675
A	1339	SER	-	expression tag	UNP P21675
A	1340	HIS	-	expression tag	UNP P21675
A	1341	MET	-	expression tag	UNP P21675

- Molecule 2 is a protein called Histone chaperone ASF1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1231	791	201	235	4			
2	D	152	Total	C	N	O	S	0	0	0
			1217	780	199	234	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q9Y294
B	-1	SER	-	expression tag	UNP Q9Y294
B	0	HIS	-	expression tag	UNP Q9Y294
D	-2	GLY	-	expression tag	UNP Q9Y294
D	-1	SER	-	expression tag	UNP Q9Y294
D	0	HIS	-	expression tag	UNP Q9Y294

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

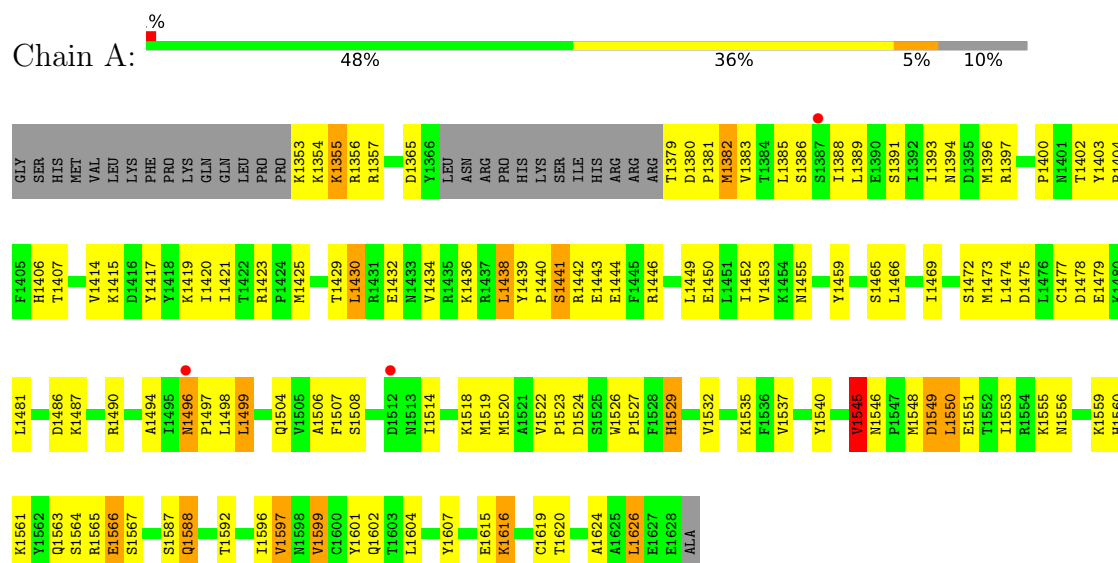


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

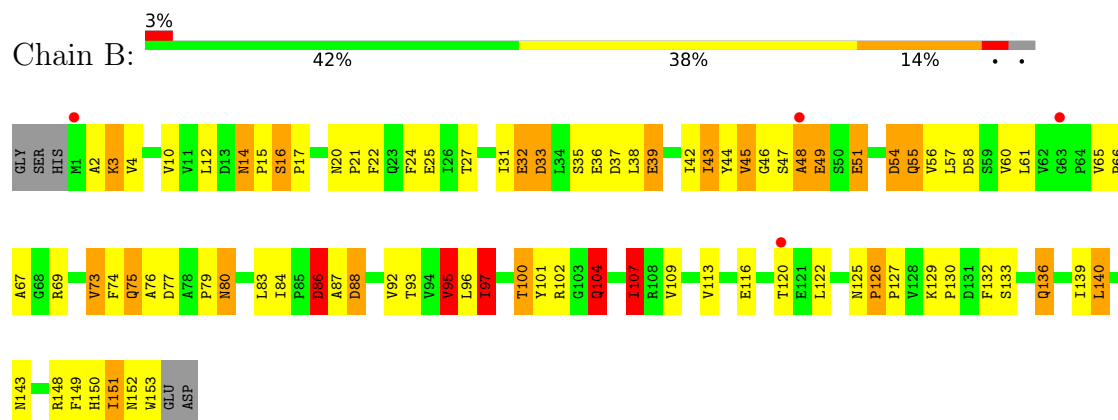
3 Residue-property plots

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: Transcription initiation factor TFIID subunit 1

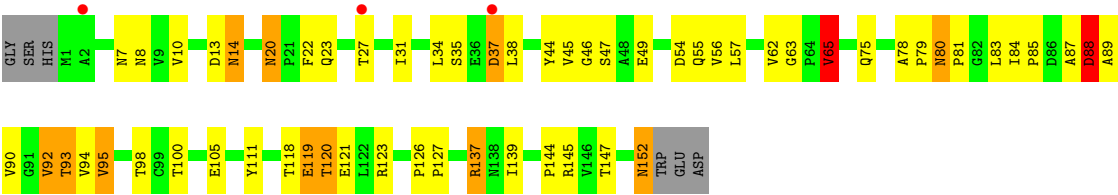


• Molecule 2: Histone chaperone ASF1A



• Molecule 2: Histone chaperone ASF1A





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.12Å 102.12Å 271.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.65 – 3.30 31.65 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (31.65-3.30) 97.2 (31.65-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.12 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.237 , 0.293 0.328 , 0.379	Depositor DCC
R_{free} test set	647 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 98.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4617	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: SO4

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	0.75	0/2206	1.10	10/2985 (0.3%)
2	B	1.43	5/1264 (0.4%)	1.35	20/1729 (1.2%)
2	D	0.71	1/1248 (0.1%)	0.96	2/1706 (0.1%)
All	All	0.97	6/4718 (0.1%)	1.14	32/6420 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	150	HIS	CE1-NE2	26.56	1.59	1.32
2	B	150	HIS	CG-ND1	19.80	1.60	1.38
2	B	150	HIS	CG-CD2	14.60	1.51	1.35
2	B	150	HIS	C-O	7.88	1.33	1.24
2	B	148	ARG	NE-CZ	6.00	1.39	1.33
2	D	152	ASN	C-O	5.33	1.34	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1496	ASN	CA-C-N	11.05	131.92	119.32
1	A	1496	ASN	C-N-CA	11.05	131.92	119.32
2	B	2	ALA	N-CA-C	8.85	122.79	108.63
2	B	150	HIS	ND1-CG-CD2	8.52	114.62	106.10
2	B	150	HIS	CG-CD2-NE2	-8.51	98.69	107.20
2	B	3	LYS	N-CA-C	8.49	120.31	111.14
2	B	16	SER	N-CA-C	7.86	115.06	108.07
2	B	37	ASP	N-CA-C	6.67	122.23	114.62
2	D	65	VAL	N-CA-C	6.45	114.50	107.60
1	A	1522	VAL	N-CA-C	6.30	114.91	107.73
2	B	20	ASN	CA-C-N	-6.19	113.30	119.99
2	B	20	ASN	C-N-CA	-6.19	113.30	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	ILE	N-CA-C	6.19	116.35	110.53
1	A	1550	LEU	N-CA-C	6.15	118.77	111.33
2	B	104	GLN	N-CA-C	6.10	118.67	108.73
1	A	1529	HIS	N-CA-C	-6.00	104.66	111.14
2	B	49	GLU	N-CA-C	5.71	120.38	113.41
1	A	1592	THR	N-CA-C	-5.64	105.05	111.14
2	B	148	ARG	N-CA-C	-5.61	98.09	107.80
2	B	97	ILE	N-CA-C	-5.54	99.90	107.99
2	B	126	PRO	CA-C-N	5.54	125.54	119.89
2	B	126	PRO	C-N-CA	5.54	125.54	119.89
1	A	1479	GLU	N-CA-C	-5.53	106.58	113.38
2	D	92	VAL	N-CA-C	5.38	115.86	108.12
1	A	1439	TYR	CA-C-N	5.32	125.40	119.87
1	A	1439	TYR	C-N-CA	5.32	125.40	119.87
1	A	1545	VAL	N-CA-C	-5.26	108.38	113.53
2	B	150	HIS	CE1-NE2-CD2	5.09	114.09	109.00
2	B	95	VAL	CB-CA-C	-5.06	102.81	110.95
2	B	80	ASN	CA-C-N	5.04	124.83	119.28
2	B	80	ASN	C-N-CA	5.04	124.83	119.28
2	B	73	VAL	CB-CA-C	-5.01	104.34	111.21

There are no chirality outliers.

There are no planarity outliers.

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	2164	0	2165	75	0
2	B	1231	0	1188	59	0
2	D	1217	0	1178	41	0
3	A	5	0	0	2	0
All	All	4617	0	4531	173	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 19.

All (173) 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:104:GLN:HG2	2:B:151:ILE:CG1	1.76	1.16
2:B:104:GLN:HG2	2:B:151:ILE:HG12	1.07	1.06
2:B:104:GLN:CG	2:B:151:ILE:HG12	1.93	0.98
2:B:95:VAL:O	2:B:96:LEU:HD23	1.69	0.91
2:B:47:SER:O	2:B:49:GLU:N	2.08	0.86
2:B:92:VAL:HA	2:B:113:VAL:O	1.80	0.81
1:A:1548:MET:O	1:A:1549:ASP:HB3	1.84	0.77
1:A:1519:MET:HE2	1:A:1550:LEU:HD21	1.67	0.75
2:B:15:PRO:HB2	2:B:136:GLN:HE22	1.53	0.73
1:A:1487:LYS:HA	1:A:1490:ARG:HB3	1.69	0.72
2:D:111:TYR:CE2	2:D:144:PRO:HG3	2.26	0.71
2:B:151:ILE:HG13	2:B:152:ASN:H	1.55	0.71
2:D:38:LEU:HD12	2:D:65:VAL:HG11	1.73	0.71
2:D:14:ASN:ND2	2:D:14:ASN:C	2.49	0.70
1:A:1472:SER:HA	1:A:1475:ASP:HB2	1.74	0.69
2:D:23:GLN:OE1	2:D:75:GLN:NE2	2.25	0.69
2:B:14:ASN:OD1	2:B:139:ILE:HB	1.94	0.67
2:B:16:SER:HB2	2:B:17:PRO:HD2	1.78	0.66
1:A:1393:ILE:HA	1:A:1396:MET:HE3	1.77	0.66
2:D:37:ASP:HB3	2:D:63:GLY:HA3	1.78	0.65
2:D:119:GLU:O	2:D:121:GLU:N	2.30	0.64
1:A:1519:MET:HE2	1:A:1550:LEU:CD2	2.27	0.64
2:D:81:PRO:HA	2:D:84:ILE:HD12	1.79	0.64
1:A:1607:TYR:CE2	2:D:145:ARG:HD3	2.33	0.64
2:B:79:PRO:HB2	2:B:84:ILE:HD11	1.80	0.64
1:A:1389:LEU:O	1:A:1393:ILE:HG13	1.98	0.64
1:A:1597:VAL:HG13	1:A:1601:TYR:CE1	2.32	0.64
2:B:22:PHE:HE2	2:B:79:PRO:HD3	1.63	0.63
2:D:20:ASN:O	2:D:137:ARG:NH2	2.25	0.63
1:A:1472:SER:C	1:A:1474:LEU:H	2.07	0.62
2:D:38:LEU:CD1	2:D:65:VAL:HG11	2.30	0.62
1:A:1497:PRO:C	1:A:1499:LEU:H	2.08	0.61
1:A:1438:LEU:O	1:A:1440:PRO:HD3	2.01	0.61
1:A:1588:GLN:HE21	1:A:1588:GLN:HA	1.66	0.61
2:B:24:PHE:CG	2:B:97:ILE:HD11	2.35	0.60
2:D:47:SER:HB2	2:D:85:PRO:HG2	1.84	0.59
1:A:1624:ALA:C	1:A:1626:LEU:H	2.10	0.59
1:A:1545:VAL:C	1:A:1546:ASN:HD22	2.11	0.59
2:B:3:LYS:HE2	2:B:153:TRP:HB3	1.85	0.59
2:B:42:ILE:HA	2:B:96:LEU:O	2.04	0.58
2:D:8:ASN:ND2	2:D:10:VAL:HG23	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1425:MET:HA	1:A:1425:MET:HE2	1.85	0.57
1:A:1472:SER:C	1:A:1474:LEU:N	2.63	0.56
1:A:1419:LYS:O	2:B:140:LEU:HD13	2.05	0.56
2:D:37:ASP:CB	2:D:63:GLY:HA3	2.35	0.56
2:B:95:VAL:C	2:B:96:LEU:HD23	2.31	0.56
2:B:4:VAL:HG21	2:B:38:LEU:HD21	1.88	0.56
2:B:15:PRO:HB2	2:B:136:GLN:NE2	2.21	0.56
2:D:8:ASN:HD21	2:D:10:VAL:HG23	1.69	0.56
2:B:39:GLU:OE2	2:B:39:GLU:HA	2.05	0.55
2:D:44:TYR:HB2	2:D:57:LEU:HD11	1.88	0.55
1:A:1417:TYR:HA	1:A:1459:TYR:CE1	2.41	0.55
1:A:1403:TYR:HA	1:A:1406:HIS:CG	2.42	0.55
2:B:32:GLU:C	2:B:33:ASP:O	2.47	0.55
1:A:1564:SER:HA	1:A:1615:GLU:HG2	1.89	0.53
2:B:151:ILE:CG1	2:B:152:ASN:H	2.21	0.53
2:D:46:GLY:H	2:D:54:ASP:HA	1.72	0.53
2:D:7:ASN:HB2	2:D:27:THR:O	2.07	0.53
2:D:14:ASN:C	2:D:14:ASN:HD22	2.14	0.53
2:B:14:ASN:ND2	2:B:15:PRO:HA	2.24	0.52
2:B:153:TRP:CD1	2:B:153:TRP:H	2.27	0.52
2:B:43:ILE:HG22	2:B:45:VAL:HG22	1.91	0.52
2:D:120:THR:HG22	2:D:123:ARG:HD2	1.91	0.52
1:A:1466:LEU:HA	1:A:1469:ILE:HG12	1.92	0.52
2:B:45:VAL:HA	2:B:54:ASP:HB3	1.91	0.52
1:A:1588:GLN:HE21	1:A:1588:GLN:CA	2.23	0.51
1:A:1397:ARG:HG3	1:A:1406:HIS:CE1	2.44	0.51
1:A:1421:ILE:HG23	1:A:1455:ASN:OD1	2.10	0.51
1:A:1430:LEU:O	1:A:1434:VAL:HG23	2.11	0.51
1:A:1449:LEU:HB3	1:A:1474:LEU:HD12	1.92	0.51
2:B:46:GLY:HA2	2:B:93:THR:HB	1.92	0.51
2:D:20:ASN:HD22	2:D:20:ASN:N	2.08	0.50
2:B:55:GLN:HE22	2:B:80:ASN:HB3	1.75	0.50
1:A:1508:SER:OG	1:A:1560:HIS:HD2	1.95	0.50
1:A:1599:VAL:HA	1:A:1602:GLN:NE2	2.27	0.50
1:A:1403:TYR:N	1:A:1404:PRO:CD	2.75	0.49
2:D:14:ASN:OD1	2:D:139:ILE:N	2.44	0.49
1:A:1396:MET:SD	1:A:1477:CYS:SG	3.11	0.49
1:A:1504:GLN:HE22	1:A:1563:GLN:HG2	1.78	0.49
2:B:51:GLU:HA	2:B:54:ASP:OD1	2.13	0.49
2:B:100:THR:HA	2:B:104:GLN:O	2.13	0.49
1:A:1466:LEU:HD23	1:A:1469:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:THR:N	2:B:113:VAL:O	2.44	0.48
1:A:1442:ARG:HG3	1:A:1443:GLU:N	2.28	0.48
2:B:75:GLN:HE21	2:B:76:ALA:N	2.12	0.48
1:A:1381:PRO:HG2	1:A:1494:ALA:O	2.14	0.48
1:A:1429:THR:HA	1:A:1432:GLU:HG2	1.96	0.48
2:B:95:VAL:HG22	2:B:113:VAL:HG21	1.96	0.48
2:D:78:ALA:HB1	2:D:79:PRO:HD2	1.95	0.47
1:A:1508:SER:OG	1:A:1560:HIS:CD2	2.68	0.47
2:B:101:TYR:N	2:B:104:GLN:O	2.40	0.47
1:A:1616:LYS:O	1:A:1619:CYS:HB2	2.14	0.47
2:B:21:PRO:HB3	2:B:77:ASP:HA	1.95	0.47
1:A:1420:ILE:HG22	1:A:1420:ILE:O	2.15	0.47
2:B:86:ASP:C	2:B:88:ASP:H	2.22	0.47
2:B:47:SER:O	2:B:48:ALA:C	2.57	0.47
2:B:104:GLN:HE21	2:B:104:GLN:N	2.13	0.47
2:D:93:THR:HB	2:D:94:VAL:H	1.56	0.47
2:B:86:ASP:C	2:B:88:ASP:N	2.73	0.46
1:A:1565:ARG:CD	1:A:1604:LEU:HD13	2.46	0.46
1:A:1587:SER:OG	1:A:1588:GLN:N	2.47	0.46
1:A:1619:CYS:O	1:A:1620:THR:C	2.59	0.46
2:D:87:ALA:C	2:D:89:ALA:H	2.22	0.46
1:A:1382:MET:HE3	1:A:1385:LEU:HD23	1.98	0.46
1:A:1477:CYS:O	1:A:1481:LEU:HG	2.16	0.46
1:A:1556:ASN:HB3	1:A:1561:LYS:HB3	1.97	0.46
2:D:31:ILE:O	2:D:31:ILE:HG22	2.16	0.46
2:B:24:PHE:CD2	2:B:97:ILE:HD11	2.51	0.46
1:A:1588:GLN:HB2	3:A:400:SO4:O1	2.15	0.46
1:A:1514:ILE:O	1:A:1518:LYS:HB2	2.16	0.45
2:B:39:GLU:OE2	2:B:61:LEU:HG	2.16	0.45
1:A:1402:THR:C	1:A:1404:PRO:HD2	2.41	0.45
2:D:121:GLU:C	2:D:123:ARG:N	2.72	0.45
3:A:400:SO4:O1	2:B:69:ARG:NH1	2.49	0.45
2:D:13:ASP:HB3	2:D:23:GLN:HG3	1.99	0.45
2:D:14:ASN:ND2	2:D:14:ASN:O	2.46	0.45
2:B:54:ASP:OD1	2:B:54:ASP:N	2.49	0.45
2:D:94:VAL:HG12	2:D:95:VAL:N	2.32	0.45
2:D:47:SER:C	2:D:49:GLU:H	2.23	0.44
2:D:34:LEU:HD12	2:D:65:VAL:HG13	1.99	0.44
2:D:37:ASP:OD2	2:D:37:ASP:N	2.50	0.44
1:A:1529:HIS:O	1:A:1551:GLU:HB2	2.18	0.44
1:A:1624:ALA:C	1:A:1626:LEU:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1526:TRP:CE3	1:A:1526:TRP:C	2.96	0.44
1:A:1532:VAL:HG11	1:A:1540:TYR:CG	2.52	0.44
1:A:1446:ARG:HG3	1:A:1478:ASP:OD1	2.18	0.44
1:A:1519:MET:CE	1:A:1550:LEU:HD21	2.41	0.44
2:B:44:TYR:HB2	2:B:57:LEU:HD11	1.99	0.43
2:B:95:VAL:HG22	2:B:113:VAL:CG2	2.48	0.43
2:B:143:ASN:O	2:B:143:ASN:OD1	2.36	0.43
1:A:1504:GLN:NE2	1:A:1563:GLN:HG2	2.33	0.43
2:D:100:THR:HA	2:D:105:GLU:HA	2.00	0.43
1:A:1526:TRP:N	1:A:1527:PRO:CD	2.81	0.43
2:B:107:ILE:CD1	2:B:109:VAL:HG23	2.48	0.43
1:A:1383:VAL:HA	1:A:1386:SER:HB2	2.00	0.43
1:A:1497:PRO:C	1:A:1499:LEU:N	2.75	0.43
1:A:1548:MET:HG3	1:A:1549:ASP:H	1.84	0.43
2:B:51:GLU:O	2:B:54:ASP:OD1	2.36	0.43
1:A:1526:TRP:CE3	1:A:1526:TRP:O	2.72	0.43
1:A:1450:GLU:HG2	1:A:1474:LEU:HD11	1.99	0.42
2:B:126:PRO:HA	2:B:127:PRO:HD2	1.70	0.42
1:A:1548:MET:HG3	1:A:1549:ASP:N	2.34	0.42
2:B:47:SER:C	2:B:49:GLU:N	2.75	0.42
2:B:10:VAL:HB	2:B:25:GLU:HB3	2.00	0.42
2:B:129:LYS:HA	2:B:130:PRO:HD3	1.88	0.42
1:A:1380:ASP:HA	1:A:1381:PRO:HD3	1.91	0.42
1:A:1565:ARG:O	1:A:1566:GLU:C	2.63	0.42
2:D:55:GLN:NE2	2:D:80:ASN:H	2.17	0.42
1:A:1565:ARG:HD2	1:A:1604:LEU:HD13	2.00	0.42
2:D:22:PHE:O	2:D:23:GLN:HG2	2.19	0.42
1:A:1417:TYR:CD2	1:A:1417:TYR:C	2.98	0.41
1:A:1550:LEU:HA	1:A:1550:LEU:HD23	1.66	0.41
2:B:33:ASP:OD1	2:B:66:PRO:HA	2.19	0.41
2:D:54:ASP:OD1	2:D:54:ASP:N	2.51	0.41
1:A:1391:SER:HA	1:A:1394:ASN:OD1	2.21	0.41
1:A:1403:TYR:HA	1:A:1406:HIS:CD2	2.56	0.41
2:B:44:TYR:CE2	2:B:79:PRO:HG3	2.55	0.41
2:B:33:ASP:HA	2:B:67:ALA:N	2.35	0.41
2:B:74:PHE:C	2:B:74:PHE:CD2	2.96	0.41
2:D:100:THR:HG23	2:D:105:GLU:N	2.35	0.41
2:B:95:VAL:CG2	2:B:113:VAL:CG2	2.98	0.41
2:D:47:SER:HA	2:D:88:ASP:CG	2.45	0.41
2:D:126:PRO:HA	2:D:127:PRO:HD2	1.94	0.41
1:A:1432:GLU:O	1:A:1436:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ILE:HD12	2:B:151:ILE:HA	1.85	0.41
1:A:1355:LYS:H	1:A:1355:LYS:HG3	1.75	0.40
1:A:1441:SER:HB3	1:A:1444:GLU:OE2	2.20	0.40
2:B:132:PHE:O	2:B:133:SER:C	2.63	0.40
2:D:31:ILE:H	2:D:31:ILE:HD12	1.86	0.40
1:A:1556:ASN:O	1:A:1560:HIS:N	2.54	0.40
1:A:1356:ARG:O	1:A:1356:ARG:HG3	2.22	0.40
1:A:1506:ALA:O	1:A:1507:PHE:C	2.64	0.40
2:D:45:VAL:HA	2:D:54:ASP:HB3	2.04	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	260/292 (89%)	218 (84%)	32 (12%)	10 (4%)	2	16
2	B	151/158 (96%)	124 (82%)	19 (13%)	8 (5%)	1	10
2	D	150/158 (95%)	125 (83%)	22 (15%)	3 (2%)	6	27
All	All	561/608 (92%)	467 (83%)	73 (13%)	21 (4%)	2	17

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1523	PRO
2	B	33	ASP
2	B	36	GLU
2	B	48	ALA
2	B	86	ASP
2	D	120	THR
1	A	1415	LYS
1	A	1498	LEU

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Mol	Chain	Res	Type
1	A	1499	LEU
1	A	1520	MET
1	A	1549	ASP
2	D	88	ASP
2	B	39	GLU
2	D	62	VAL
1	A	1400	PRO
1	A	1566	GLU
1	A	1473	MET
1	A	1596	ILE
2	B	87	ALA
2	B	102	ARG
2	B	107	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	250/276 (91%)	218 (87%)	32 (13%)	4	18
2	B	138/142 (97%)	106 (77%)	32 (23%)	1	4
2	D	137/142 (96%)	118 (86%)	19 (14%)	3	15
All	All	525/560 (94%)	442 (84%)	83 (16%)	2	12

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1353	LYS
1	A	1354	LYS
1	A	1355	LYS
1	A	1357	ARG
1	A	1365	ASP
1	A	1379	THR
1	A	1382	MET
1	A	1388	ILE
1	A	1407	THR

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Mol	Chain	Res	Type
1	A	1414	VAL
1	A	1423	ARG
1	A	1430	LEU
1	A	1438	LEU
1	A	1441	SER
1	A	1452	ILE
1	A	1453	VAL
1	A	1465	SER
1	A	1486	ASP
1	A	1496	ASN
1	A	1524	ASP
1	A	1535	LYS
1	A	1537	VAL
1	A	1545	VAL
1	A	1553	ILE
1	A	1555	LYS
1	A	1559	LYS
1	A	1567	SER
1	A	1588	GLN
1	A	1597	VAL
1	A	1599	VAL
1	A	1616	LYS
1	A	1626	LEU
2	B	12	LEU
2	B	14	ASN
2	B	27	THR
2	B	32	GLU
2	B	35	SER
2	B	43	ILE
2	B	45	VAL
2	B	51	GLU
2	B	54	ASP
2	B	55	GLN
2	B	56	VAL
2	B	58	ASP
2	B	60	VAL
2	B	65	VAL
2	B	73	VAL
2	B	75	GLN
2	B	83	LEU
2	B	86	ASP
2	B	88	ASP

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Mol	Chain	Res	Type
2	B	95	VAL
2	B	97	ILE
2	B	100	THR
2	B	104	GLN
2	B	107	ILE
2	B	116	GLU
2	B	120	THR
2	B	122	LEU
2	B	125	ASN
2	B	136	GLN
2	B	140	LEU
2	B	149	PHE
2	B	151	ILE
2	D	14	ASN
2	D	20	ASN
2	D	35	SER
2	D	37	ASP
2	D	56	VAL
2	D	65	VAL
2	D	80	ASN
2	D	83	LEU
2	D	88	ASP
2	D	90	VAL
2	D	92	VAL
2	D	93	THR
2	D	95	VAL
2	D	98	THR
2	D	118	THR
2	D	119	GLU
2	D	137	ARG
2	D	147	THR
2	D	152	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1406	HIS
1	A	1448	HIS
1	A	1464	HIS
1	A	1468	GLN
1	A	1496	ASN
1	A	1504	GLN

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Mol	Chain	Res	Type
1	A	1513	ASN
1	A	1529	HIS
1	A	1546	ASN
1	A	1560	HIS
1	A	1588	GLN
1	A	1602	GLN
2	B	20	ASN
2	B	55	GLN
2	B	75	GLN
2	B	104	GLN
2	B	136	GLN
2	B	138	ASN
2	B	143	ASN
2	D	7	ASN
2	D	8	ASN
2	D	20	ASN
2	D	55	GLN
2	D	115	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	SO4	A	400	-	4,4,4	0.56	0	6,6,6	0.28	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	SO4	2	0

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	264/292 (90%)	0.10	3 (1%) 78 60	40, 40, 40, 40	0
2	B	153/158 (96%)	0.27	4 (2%) 57 38	40, 40, 40, 40	0
2	D	152/158 (96%)	0.26	3 (1%) 65 46	40, 40, 40, 40	0
All	All	569/608 (93%)	0.19	10 (1%) 67 49	40, 40, 40, 40	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	2.6
2	B	120	THR	2.4
1	A	1512	ASP	2.4
2	D	37	ASP	2.3
2	B	63	GLY	2.3
1	A	1387	SER	2.3
2	D	2	ALA	2.2
2	D	27	THR	2.2
1	A	1496	ASN	2.1
2	B	48	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	400	5/5	0.92	0.30	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.