Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 04:46 AM EST

PDB ID	:	3O37
Title	:	Crystal structure of TRIM24 PHD-Bromo complexed with H3(1-10)K4 peptide
Authors	:	Wang, Z.; Patel, D.J.
Deposited on	:	2010-07-23
Resolution	:	2.00 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:

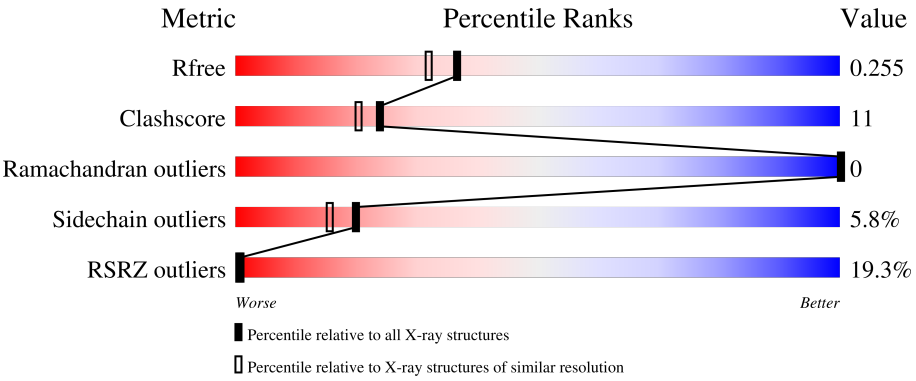
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	184	18% 73% 21% • 5%
1	B	184	16% 77% 18% • •
1	C	184	14% 73% 22% • •
1	D	184	19% 68% 24% • 5%
2	E	10	30% 70% 30%

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Mol	Chain	Length	Quality of chain
2	F	10	
2	G	10	
2	H	10	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6308 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 intermediary factor 1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1428	916	227	270	15			
1	B	180	Total	C	N	O	S	0	0	0
			1462	935	233	279	15			
1	C	176	Total	C	N	O	S	0	0	0
			1435	921	228	271	15			
1	D	174	Total	C	N	O	S	0	0	0
			1419	911	226	267	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	823	SER	-	expression tag	UNP O15164
B	823	SER	-	expression tag	UNP O15164
C	823	SER	-	expression tag	UNP O15164
D	823	SER	-	expression tag	UNP O15164

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	0	0	0
			80	46	19	15			
2	F	10	Total	C	N	O	0	0	0
			80	46	19	15			
2	G	10	Total	C	N	O	0	0	0
			80	46	19	15			
2	H	10	Total	C	N	O	0	0	0
			80	46	19	15			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0

- Molecule 4 is water.

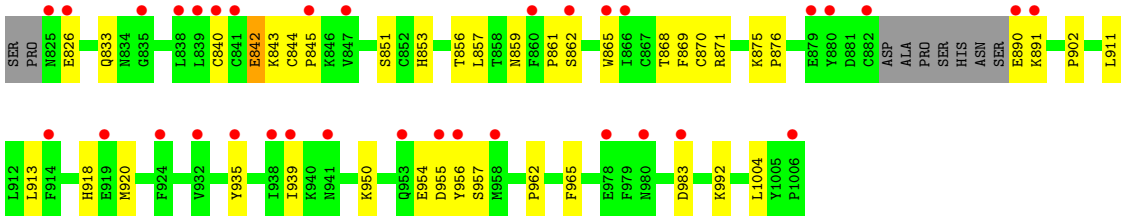
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	59	Total O 59 59	0	0
4	B	57	Total O 57 57	0	0
4	C	54	Total O 54 54	0	0
4	D	66	Total O 66 66	0	0

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.

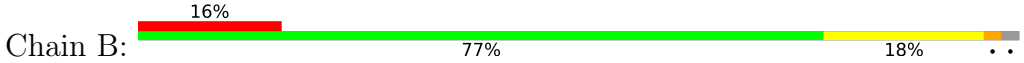
• Molecule 1: Transcription intermediary factor 1-alpha

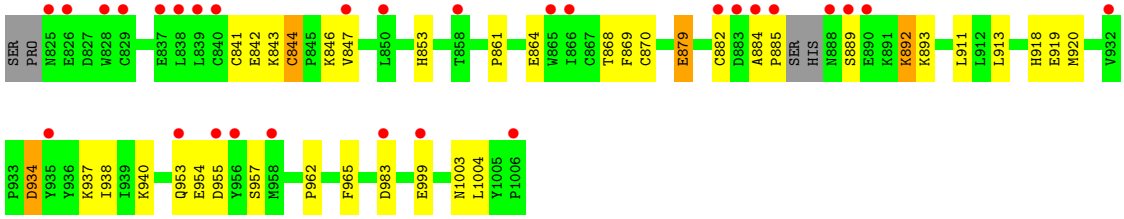
Chain A:



• Molecule 1: Transcription intermediary factor 1-alpha

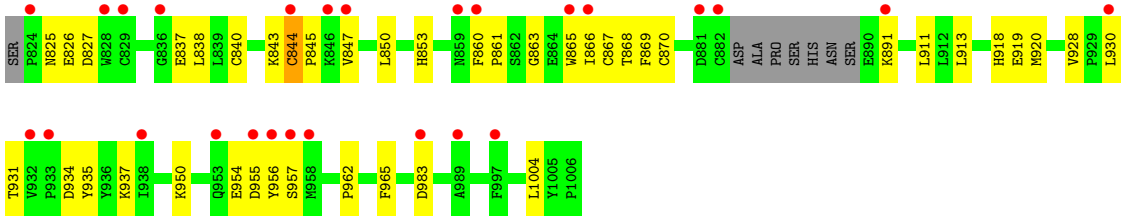
Chain B:





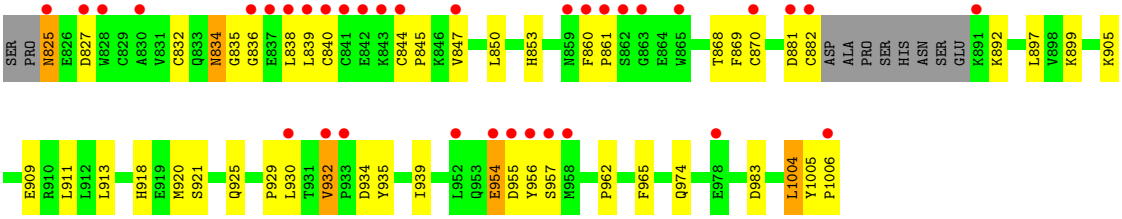
• Molecule 1: Transcription intermediary factor 1-alpha

Chain C:

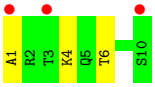


• Molecule 1: Transcription intermediary factor 1-alpha

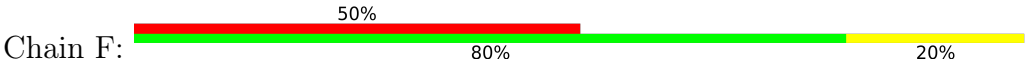
Chain D:

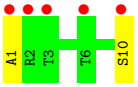


• Molecule 2: Histone H3.1

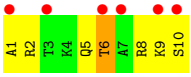


• Molecule 2: Histone H3.1

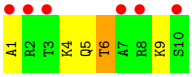




• Molecule 2: Histone H3.1



• Molecule 2: Histone H3.1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	35.67Å 63.85Å 79.30Å 89.92° 89.99° 89.80°	Depositor
Resolution (Å)	35.67 – 2.00 35.67 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.6 (35.67-2.00) 96.9 (35.67-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.254 0.227 , 0.255	Depositor DCC
R_{free} test set	2787 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 29.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l 0.437 for -h,k,-l 0.430 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6308	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.35	0/1463	0.59	0/1977
1	B	0.37	0/1498	0.60	0/2026
1	C	0.35	0/1471	0.59	0/1988
1	D	0.34	0/1454	0.58	0/1965
2	E	0.36	0/79	0.68	0/101
2	F	0.36	0/79	0.61	0/101
2	G	0.37	0/79	0.69	0/101
2	H	0.34	0/79	0.61	0/101
All	All	0.35	0/6202	0.59	0/8360

There are no bond length outliers.

There are no bond angle outliers.

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	1428	0	1388	28	0
1	B	1462	0	1415	32	0
1	C	1435	0	1396	37	0
1	D	1419	0	1382	45	0
2	E	80	0	91	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	80	0	91	4	0
2	G	80	0	91	9	0
2	H	80	0	91	9	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	59	0	0	1	0
4	B	57	0	0	2	0
4	C	54	0	0	1	0
4	D	66	0	0	1	0
All	All	6308	0	5945	133	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 11.

All (133) 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:C:861:PRO:HG2	2:G:1:ALA:HB2	1.44	0.96
1:A:861:PRO:HG2	2:E:1:ALA:HB2	1.48	0.94
1:B:861:PRO:HG2	2:F:1:ALA:HB2	1.53	0.89
1:C:838:LEU:HB3	1:C:847:VAL:HG22	1.54	0.88
1:C:861:PRO:HG2	2:G:1:ALA:CB	2.06	0.85
1:C:853:HIS:HE1	1:C:868:THR:H	1.24	0.84
1:D:827:ASP:HB3	2:H:6:THR:HG21	1.66	0.78
1:B:853:HIS:HE1	1:B:868:THR:H	1.29	0.77
1:A:853:HIS:HE1	1:A:868:THR:H	1.30	0.77
1:C:827:ASP:O	2:G:6:THR:HG21	1.86	0.76
1:B:918:HIS:HD2	1:B:920:MET:H	1.32	0.76
1:C:825:ASN:HD21	2:G:2:ARG:HH21	1.31	0.76
1:D:838:LEU:HD23	1:D:847:VAL:HG21	1.69	0.75
1:C:957:SER:HB3	4:C:130:HOH:O	1.87	0.74
1:D:853:HIS:HE1	1:D:868:THR:H	1.33	0.74
1:D:834:ASN:ND2	1:D:835:GLY:H	1.87	0.72
1:B:842:GLU:OE2	1:B:864:GLU:HG3	1.91	0.71
1:D:918:HIS:HD2	1:D:920:MET:H	1.39	0.70
1:C:838:LEU:HB3	1:C:847:VAL:CG2	2.21	0.70
1:C:825:ASN:ND2	2:G:2:ARG:HH21	1.90	0.69
1:B:879:GLU:OE2	1:B:884:ALA:HA	1.94	0.68
1:B:879:GLU:OE2	1:B:884:ALA:CA	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:PRO:HG2	2:E:1:ALA:CB	2.23	0.65
1:B:918:HIS:CD2	1:B:920:MET:H	2.12	0.65
1:B:853:HIS:CE1	1:B:868:THR:H	2.12	0.65
1:D:834:ASN:HD22	1:D:835:GLY:H	1.44	0.65
1:D:861:PRO:HB2	2:H:1:ALA:HB2	1.79	0.65
1:B:892:LYS:HE2	4:B:153:HOH:O	1.96	0.64
1:D:911:LEU:HG	1:D:1004:LEU:HD23	1.80	0.64
1:C:837:GLU:HG3	2:G:5:GLN:HE22	1.62	0.63
2:G:9:LYS:O	2:G:10:SER:HB2	1.99	0.63
1:D:834:ASN:HD21	2:H:9:LYS:H	1.46	0.62
1:B:861:PRO:O	2:F:1:ALA:HB2	2.01	0.61
1:D:825:ASN:N	1:D:825:ASN:HD22	1.98	0.61
1:A:875:LYS:HE2	1:B:999:GLU:CD	2.20	0.60
1:C:918:HIS:CD2	1:C:920:MET:H	2.19	0.60
1:B:940:LYS:HG2	1:C:863:GLY:HA2	1.84	0.60
1:D:825:ASN:N	1:D:825:ASN:ND2	2.47	0.60
1:B:861:PRO:HG2	2:F:1:ALA:CB	2.30	0.60
1:A:861:PRO:O	2:E:1:ALA:HB2	2.01	0.59
1:A:840:CYS:SG	2:E:4:LYS:HB2	2.43	0.59
1:C:918:HIS:HD2	1:C:920:MET:H	1.48	0.59
1:B:844:CYS:HB3	1:B:870:CYS:SG	2.44	0.58
1:C:853:HIS:CE1	1:C:868:THR:H	2.13	0.58
1:D:836:GLY:O	1:D:838:LEU:HD13	2.04	0.58
1:D:918:HIS:CD2	1:D:920:MET:H	2.20	0.58
1:C:930:LEU:O	1:D:920:MET:HE1	2.04	0.57
1:D:892:LYS:HE3	4:D:146:HOH:O	2.03	0.57
1:A:918:HIS:HD2	1:A:920:MET:H	1.50	0.57
1:C:962:PRO:HA	1:C:965:PHE:CE2	2.40	0.56
1:B:869:PHE:CZ	1:B:913:LEU:HG	2.41	0.55
1:C:844:CYS:HB3	1:C:870:CYS:SG	2.46	0.55
1:B:962:PRO:HA	1:B:965:PHE:CE2	2.41	0.55
1:D:834:ASN:HD22	1:D:835:GLY:N	2.05	0.54
1:A:918:HIS:CD2	1:A:920:MET:H	2.25	0.54
1:C:911:LEU:HG	1:C:1004:LEU:HD12	1.89	0.54
1:A:962:PRO:HA	1:A:965:PHE:CE2	2.43	0.54
1:A:859:ASN:HB2	1:D:974:GLN:NE2	2.22	0.54
1:B:934:ASP:HA	1:B:937:LYS:HD2	1.89	0.54
1:D:834:ASN:ND2	2:H:9:LYS:H	2.06	0.54
1:D:869:PHE:CZ	1:D:913:LEU:HG	2.42	0.53
1:C:850:LEU:HD21	1:C:860:PHE:CE2	2.44	0.53
1:B:911:LEU:HG	1:B:1004:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:962:PRO:HA	1:D:965:PHE:CE2	2.44	0.52
1:D:844:CYS:HB3	1:D:870:CYS:SG	2.51	0.52
4:A:147:HOH:O	1:D:974:GLN:HG2	2.10	0.51
1:B:919:GLU:HG3	1:B:920:MET:HE2	1.93	0.51
1:B:919:GLU:HG3	1:B:920:MET:CE	2.41	0.51
1:C:931:THR:HA	1:D:920:MET:HE3	1.93	0.51
1:A:851:SER:HA	1:A:856:THR:HG23	1.93	0.50
1:C:911:LEU:HG	1:C:1004:LEU:CD1	2.42	0.50
1:D:825:ASN:N	1:D:845:PRO:O	2.44	0.50
1:C:937:LYS:HE3	1:D:832:CYS:HB2	1.92	0.50
1:D:881:ASP:OD1	1:D:882:CYS:N	2.45	0.50
1:A:853:HIS:CE1	1:A:868:THR:H	2.21	0.50
1:D:853:HIS:CE1	1:D:868:THR:H	2.23	0.50
1:D:929:PRO:O	1:D:932:VAL:HG23	2.11	0.50
2:H:5:GLN:HA	2:H:5:GLN:OE1	2.11	0.50
1:C:937:LYS:CE	1:D:832:CYS:HB2	2.42	0.49
1:D:838:LEU:HD23	1:D:847:VAL:CG2	2.40	0.49
1:D:827:ASP:CB	2:H:6:THR:HG21	2.41	0.49
1:B:882:CYS:HB2	1:B:953:GLN:NE2	2.28	0.49
1:C:825:ASN:HD21	2:G:2:ARG:NH2	2.06	0.48
1:C:861:PRO:O	2:G:1:ALA:HB2	2.13	0.48
1:C:956:TYR:O	1:C:957:SER:C	2.52	0.48
1:A:862:SER:OG	1:D:974:GLN:HG3	2.14	0.48
1:A:859:ASN:HB2	1:D:974:GLN:HE22	1.79	0.47
1:A:992:LYS:HE2	1:A:992:LYS:HB3	1.69	0.47
1:B:861:PRO:CG	2:F:1:ALA:HB2	2.36	0.47
1:D:954:GLU:HA	1:D:954:GLU:OE2	2.15	0.46
1:A:902:PRO:HD2	1:B:1003:ASN:HA	1.97	0.46
1:A:911:LEU:HG	1:A:1004:LEU:HD12	1.97	0.46
1:D:861:PRO:O	2:H:1:ALA:HB2	2.15	0.46
1:C:869:PHE:CZ	1:C:913:LEU:HG	2.50	0.46
1:A:869:PHE:CZ	1:A:913:LEU:HG	2.50	0.46
1:A:859:ASN:CB	1:D:974:GLN:NE2	2.79	0.46
1:C:919:GLU:HG3	1:C:920:MET:N	2.31	0.46
1:B:841:CYS:SG	1:B:842:GLU:N	2.89	0.45
1:C:838:LEU:CB	1:C:847:VAL:CG2	2.94	0.45
1:C:928:VAL:HG21	1:C:935:TYR:CZ	2.52	0.45
1:D:905:LYS:O	1:D:909:GLU:HG3	2.17	0.45
1:B:957:SER:HB2	4:B:145:HOH:O	2.16	0.45
1:B:843:LYS:HA	1:B:843:LYS:HD3	1.74	0.44
1:D:850:LEU:HD11	1:D:860:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:GLU:HG2	1:A:865:TRP:O	2.17	0.44
1:C:843:LYS:HG2	1:C:866:ILE:HD12	1.99	0.44
1:D:840:CYS:SG	2:H:4:LYS:HG3	2.57	0.44
1:D:921:SER:O	1:D:925:GLN:HG3	2.17	0.44
1:D:930:LEU:C	1:D:932:VAL:H	2.20	0.44
1:B:844:CYS:SG	1:B:846:LYS:CG	3.06	0.43
1:B:892:LYS:HD3	1:B:893:LYS:N	2.33	0.43
1:A:935:TYR:CZ	1:A:939:ILE:HG13	2.53	0.43
1:B:934:ASP:O	1:B:938:ILE:HG13	2.18	0.43
1:B:879:GLU:OE2	1:B:884:ALA:N	2.52	0.43
1:D:935:TYR:CZ	1:D:939:ILE:HG13	2.53	0.43
1:D:956:TYR:O	1:D:957:SER:C	2.57	0.42
1:A:844:CYS:HB3	1:A:870:CYS:SG	2.59	0.42
1:C:950:LYS:HB2	1:C:950:LYS:NZ	2.35	0.42
1:A:833:GLN:NE2	1:A:833:GLN:HA	2.34	0.42
1:C:919:GLU:HG3	1:C:920:MET:HE2	2.00	0.42
1:D:1005:TYR:N	1:D:1006:PRO:HD3	2.35	0.42
1:C:826:GLU:HG3	1:C:845:PRO:O	2.19	0.42
1:A:826:GLU:HB2	1:A:845:PRO:O	2.20	0.42
1:C:865:TRP:CH2	1:C:867:CYS:HA	2.55	0.42
1:C:825:ASN:OD1	1:C:840:CYS:HB3	2.20	0.41
1:A:861:PRO:CG	2:E:1:ALA:HB2	2.35	0.41
1:A:956:TYR:O	1:A:957:SER:C	2.58	0.41
1:B:911:LEU:HG	1:B:1004:LEU:CD1	2.50	0.41
1:D:825:ASN:O	2:H:4:LYS:NZ	2.53	0.41
1:C:937:LYS:HB3	1:C:937:LYS:NZ	2.36	0.41
1:A:911:LEU:HG	1:A:1004:LEU:CD1	2.51	0.41
1:A:871:ARG:HD2	1:A:876:PRO:HB3	2.03	0.40
1:B:884:ALA:HA	1:B:885:PRO:HD2	1.89	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	171/184 (93%)	167 (98%)	4 (2%)	0	100	100
1	B	176/184 (96%)	172 (98%)	4 (2%)	0	100	100
1	C	172/184 (94%)	167 (97%)	5 (3%)	0	100	100
1	D	170/184 (92%)	165 (97%)	5 (3%)	0	100	100
2	E	8/10 (80%)	8 (100%)	0	0	100	100
2	F	8/10 (80%)	8 (100%)	0	0	100	100
2	G	8/10 (80%)	8 (100%)	0	0	100	100
2	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	721/776 (93%)	702 (97%)	19 (3%)	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	164/172 (95%)	155 (94%)	9 (6%)	21	17
1	B	168/172 (98%)	159 (95%)	9 (5%)	22	18
1	C	165/172 (96%)	159 (96%)	6 (4%)	35	34
1	D	163/172 (95%)	152 (93%)	11 (7%)	16	11
2	E	8/8 (100%)	7 (88%)	1 (12%)	4	2
2	F	8/8 (100%)	7 (88%)	1 (12%)	4	2
2	G	8/8 (100%)	6 (75%)	2 (25%)	0	0
2	H	8/8 (100%)	7 (88%)	1 (12%)	4	2
All	All	692/720 (96%)	652 (94%)	40 (6%)	20	15

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	842	GLU
1	A	843	LYS

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Mol	Chain	Res	Type
1	A	857	LEU
1	A	890	GLU
1	A	891	LYS
1	A	950	LYS
1	A	954	GLU
1	A	955	ASP
1	A	983	ASP
1	B	844	CYS
1	B	847	VAL
1	B	879	GLU
1	B	889	SER
1	B	892	LYS
1	B	934	ASP
1	B	954	GLU
1	B	955	ASP
1	B	983	ASP
1	C	844	CYS
1	C	891	LYS
1	C	934	ASP
1	C	954	GLU
1	C	955	ASP
1	C	983	ASP
1	D	825	ASN
1	D	834	ASN
1	D	839	LEU
1	D	897	LEU
1	D	899	LYS
1	D	932	VAL
1	D	934	ASP
1	D	954	GLU
1	D	955	ASP
1	D	983	ASP
1	D	1004	LEU
2	E	6	THR
2	F	10	SER
2	G	6	THR
2	G	8	ARG
2	H	6	THR

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	833	GLN
1	A	853	HIS
1	A	918	HIS
1	A	974	GLN
1	B	825	ASN
1	B	853	HIS
1	B	918	HIS
1	B	974	GLN
1	C	825	ASN
1	C	853	HIS
1	C	918	HIS
1	C	974	GLN
1	C	1003	ASN
1	D	834	ASN
1	D	853	HIS
1	D	918	HIS
1	D	1003	ASN
2	G	5	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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, 95^{th} 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	175/184 (95%)	1.36	34 (19%)	1	0	20, 36, 74, 115	0
1	B	180/184 (97%)	1.28	29 (16%)	1	1	21, 36, 85, 106	0
1	C	176/184 (95%)	1.21	26 (14%)	2	2	21, 36, 71, 106	0
1	D	174/184 (94%)	1.27	35 (20%)	1	0	21, 36, 72, 103	0
2	E	10/10 (100%)	2.27	3 (30%)	0	0	66, 74, 78, 92	0
2	F	10/10 (100%)	3.49	5 (50%)	0	0	62, 69, 78, 90	0
2	G	10/10 (100%)	3.18	6 (60%)	0	0	69, 72, 85, 95	0
2	H	10/10 (100%)	2.85	6 (60%)	0	0	65, 70, 78, 93	0
All	All	745/776 (96%)	1.37	144 (19%)	1	0	20, 37, 77, 115	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	956	TYR	17.3
1	B	956	TYR	17.2
2	F	1	ALA	14.8
1	D	956	TYR	14.5
1	A	955	ASP	13.5
1	B	955	ASP	12.7
1	A	882	CYS	9.5
1	C	956	TYR	9.3
1	D	882	CYS	8.4
1	C	955	ASP	8.2
2	G	10	SER	7.6
1	B	885	PRO	6.9
1	B	888	ASN	6.2
2	E	10	SER	6.1
1	C	824	PRO	5.9
1	C	933	PRO	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	983	ASP	5.7
1	C	891	LYS	5.7
2	H	10	SER	5.6
1	A	835	GLY	5.6
1	B	828	TRP	5.3
1	C	882	CYS	5.3
1	D	955	ASP	5.1
2	F	3	THR	5.0
1	D	933	PRO	4.9
2	H	1	ALA	4.7
1	A	866	ILE	4.7
1	B	837	GLU	4.7
2	H	3	THR	4.6
2	G	1	ALA	4.6
2	F	10	SER	4.4
1	D	828	TRP	4.4
2	E	3	THR	4.4
1	A	862	SER	4.1
1	B	889	SER	4.1
1	D	1006	PRO	4.1
1	C	828	TRP	4.0
2	G	9	LYS	4.0
2	E	1	ALA	4.0
1	C	983	ASP	4.0
1	A	860	PHE	4.0
2	F	2	ARG	3.9
1	C	881	ASP	3.8
2	H	7	ALA	3.8
1	A	839	LEU	3.8
1	D	838	LEU	3.8
1	D	840	CYS	3.7
1	C	866	ILE	3.7
1	A	935	TYR	3.7
1	D	932	VAL	3.7
1	A	847	VAL	3.6
1	A	932	VAL	3.6
2	G	3	THR	3.5
1	B	839	LEU	3.5
1	D	839	LEU	3.5
1	D	847	VAL	3.5
1	C	836	GLY	3.4
1	C	930	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	891	LYS	3.3
1	B	825	ASN	3.3
1	D	836	GLY	3.3
1	A	1006	PRO	3.3
1	D	825	ASN	3.2
1	C	953	GLN	3.2
1	B	932	VAL	3.2
1	C	846	LYS	3.1
2	G	7	ALA	3.1
1	B	826	GLU	3.1
1	A	983	ASP	3.1
1	D	827	ASP	3.1
1	D	865	TRP	3.0
1	C	865	TRP	3.0
1	C	860	PHE	3.0
1	D	841	CYS	3.0
1	D	842	GLU	3.0
1	A	865	TRP	2.9
1	A	845	PRO	2.9
1	D	844	CYS	2.9
1	A	826	GLU	2.9
1	A	939	ILE	2.9
1	C	829	CYS	2.9
2	F	6	THR	2.9
2	H	8	ARG	2.9
1	B	890	GLU	2.8
1	B	884	ALA	2.8
1	B	883	ASP	2.8
1	A	880	TYR	2.8
1	B	865	TRP	2.7
1	D	881	ASP	2.7
1	D	958	MET	2.7
1	C	932	VAL	2.7
1	D	859	ASN	2.7
1	A	891	LYS	2.6
1	A	879	GLU	2.6
1	D	830	ALA	2.6
1	A	924	PHE	2.6
1	D	952	LEU	2.5
1	A	914	PHE	2.5
1	C	844	CYS	2.5
1	B	858	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	6	THR	2.5
1	D	863	GLY	2.5
1	A	825	ASN	2.5
1	C	957	SER	2.5
1	D	860	PHE	2.5
1	A	958	MET	2.4
1	D	837	GLU	2.4
1	D	954	GLU	2.4
1	B	866	ILE	2.4
1	D	861	PRO	2.4
1	B	958	MET	2.4
2	H	2	ARG	2.4
1	B	882	CYS	2.3
1	B	1006	PRO	2.3
1	A	980	ASN	2.3
1	A	838	LEU	2.3
1	B	850	LEU	2.3
1	B	847	VAL	2.3
1	C	847	VAL	2.3
1	B	840	CYS	2.3
1	C	989	ALA	2.3
1	C	859	ASN	2.2
1	C	958	MET	2.2
1	D	930	LEU	2.2
1	B	935	TYR	2.2
1	B	953	GLN	2.2
1	A	890	GLU	2.2
1	A	938	ILE	2.2
1	A	941	ASN	2.2
1	B	999	GLU	2.2
1	A	841	CYS	2.2
1	C	997	PHE	2.2
1	D	870	CYS	2.1
1	D	862	SER	2.1
1	A	919	GLU	2.1
1	D	843	LYS	2.1
1	B	829	CYS	2.1
1	C	938	ILE	2.1
1	A	978	GLU	2.1
1	D	978	GLU	2.1
1	D	957	SER	2.0
1	A	840	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	838	LEU	2.0
1	A	953	GLN	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 monosaccharides 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, 95^{th} 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	ZN	D	1	1/1	0.88	0.11	45,45,45,45	0
3	ZN	A	1	1/1	0.89	0.09	46,46,46,46	0
3	ZN	A	2	1/1	0.90	0.05	46,46,46,46	0
3	ZN	D	2	1/1	0.90	0.15	46,46,46,46	0
3	ZN	B	1	1/1	0.93	0.13	45,45,45,45	0
3	ZN	B	2	1/1	0.96	0.12	49,49,49,49	0
3	ZN	C	1	1/1	0.96	0.14	45,45,45,45	0
3	ZN	C	2	1/1	0.97	0.16	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.