Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:27 PM GMT

PDB ID	:	4OY2
Title	:	Crystal structure of TAF1-TAF7, a TFIID subcomplex
Authors	:	Bhattacharya, S.; Lou, X.; Rajashankar, K.; Jacobson, R.H.; Webb, P.
Deposited on	:	2014-02-10
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

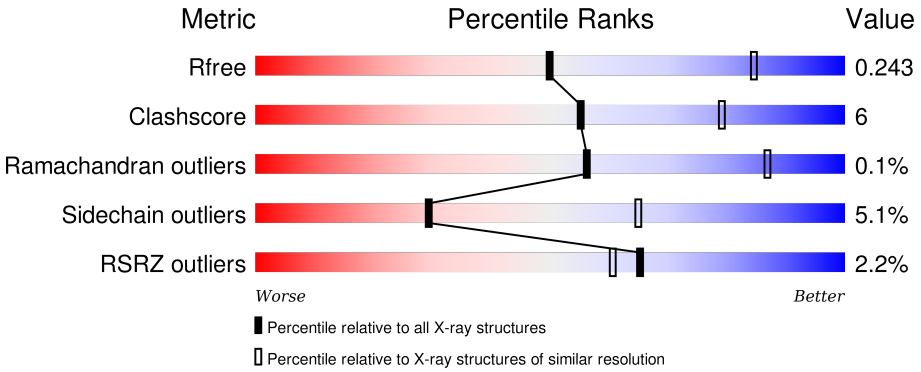
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	506	76% 16% • 7%
1	C	506	6% 78% 12% • 9%
1	E	506	% 72% 18% • 8%
2	B	235	77% 19% • •
2	D	235	3% 77% 18% •

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Mol	Chain	Length	Quality of chain
2	F	235	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16474 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	470	Total	C	N	O	S	Se	0	3	0
			3726	2358	660	696	1	11			
1	C	460	Total	C	N	O	S	Se	0	2	0
			3526	2231	619	664	1	11			
1	E	468	Total	C	N	O	S	Se	0	8	0
			3787	2401	670	704	1	11			

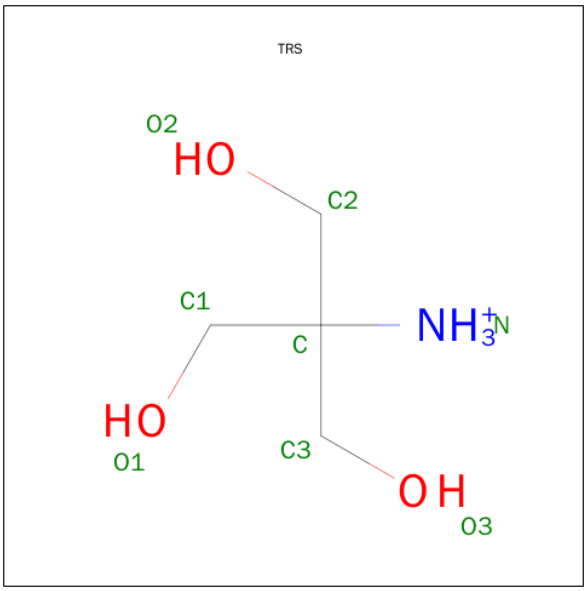
- Molecule 2 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	Se	0	0	0
			1825	1157	301	361	1	5			
2	D	225	Total	C	N	O	S	Se	0	1	0
			1774	1123	295	350	1	5			
2	F	225	Total	C	N	O	S	Se	0	3	0
			1814	1149	298	361	1	5			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is water.

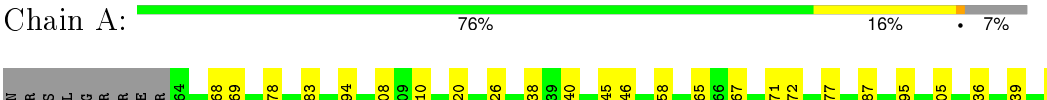
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	C	2	Total O 2 2	0	0
5	E	5	Total O 5 5	0	0
5	D	2	Total O 2 2	0	0
5	F	1	Total O 1 1	0	0

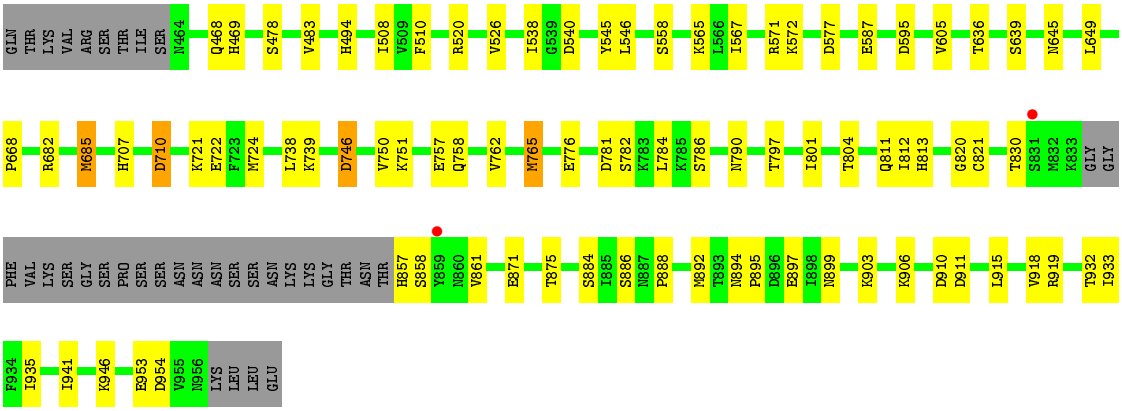
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Transcription initiation factor TFIID subunit 1

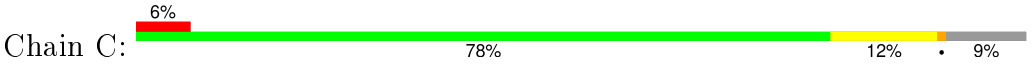
Chain A:

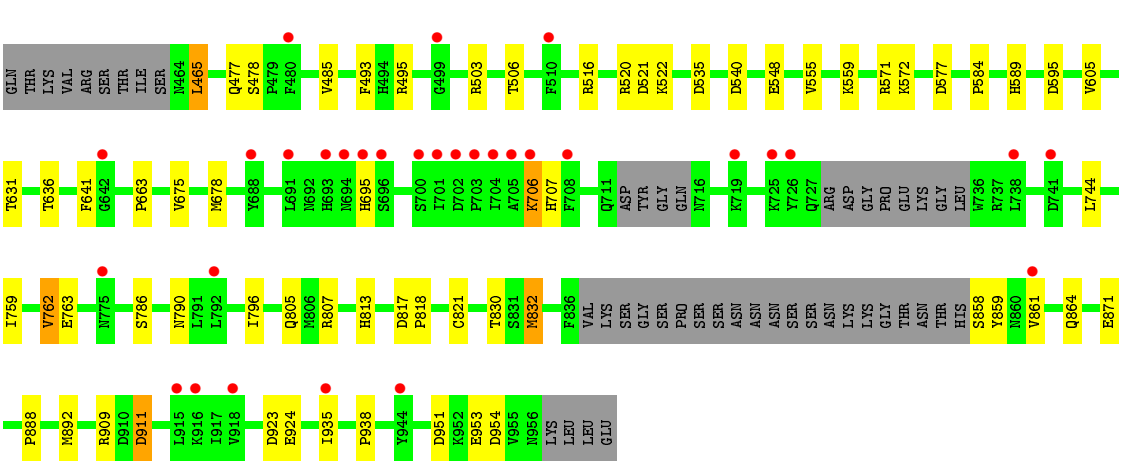




- Molecule 1: Transcription initiation factor TFIID subunit 1

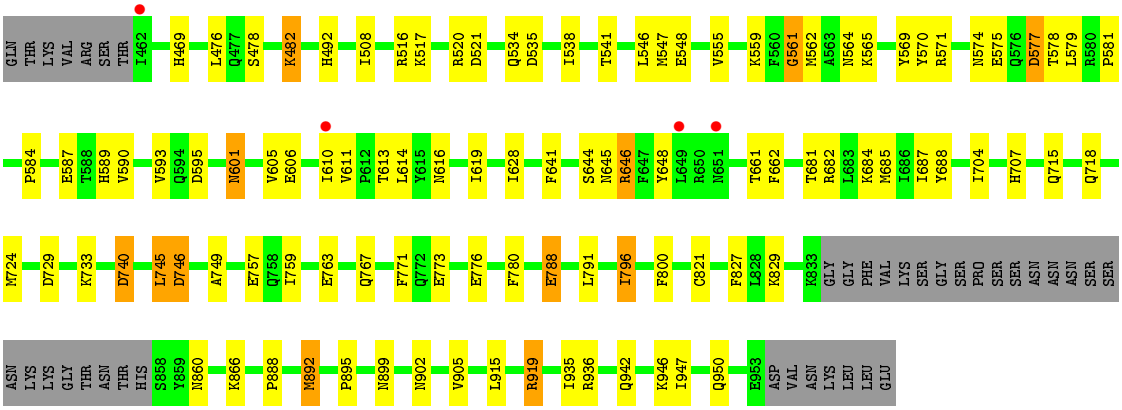
Chain C:





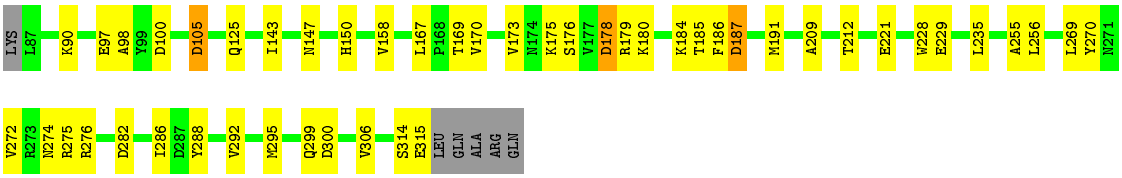
- Molecule 1: Transcription initiation factor TFIID subunit 1

Chain E:



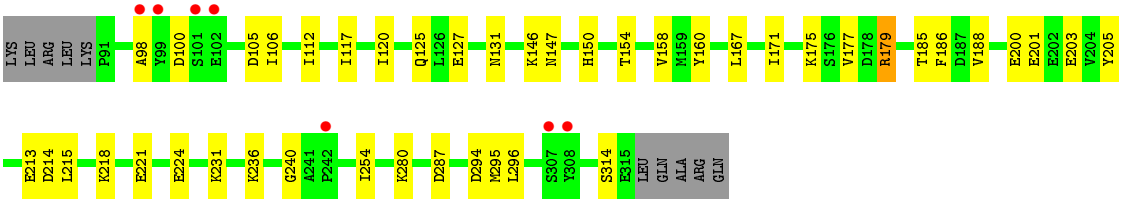
• Molecule 2: Transcription initiation factor TFIID subunit 7

Chain B:



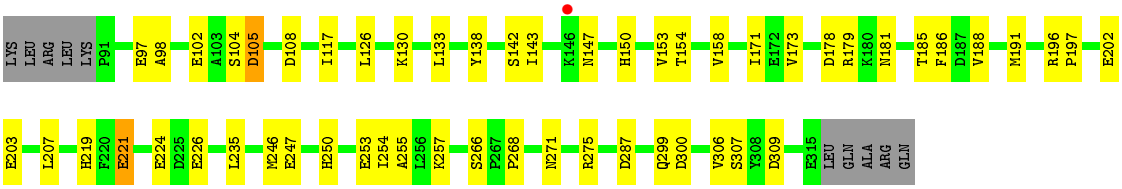
• Molecule 2: Transcription initiation factor TFIID subunit 7

Chain D:



• Molecule 2: Transcription initiation factor TFIID subunit 7

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.22Å 123.66Å 229.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.68 – 2.90 84.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (83.68-2.90) 99.9 (84.14-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.209 , 0.243 0.207 , 0.243	Depositor DCC
R_{free} test set	3931 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	70.6	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.9	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 77943 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16474	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, TRS

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	0.26	0/3809	0.44	0/5140
1	C	0.25	0/3598	0.44	0/4861
1	E	0.27	0/3884	0.44	0/5227
2	B	0.25	0/1853	0.44	0/2502
2	D	0.25	0/1804	0.46	0/2439
2	F	0.26	0/1850	0.43	0/2496
All	All	0.26	0/16798	0.44	0/22665

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	3726	0	3572	50	0
1	C	3526	0	3290	36	0
1	E	3787	0	3713	64	0
2	B	1825	0	1781	34	0
2	D	1774	0	1704	25	0
2	F	1814	0	1776	35	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	12	1	0
5	A	3	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	5	0	0	0	0
5	F	1	0	0	0	0
All	All	16474	0	15848	204	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 6.

All (204) 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:832:MSE:HG2	1:C:861:VAL:HG12	1.56	0.88
1:E:682:ARG:NH1	2:F:98:ALA:O	2.22	0.73
1:A:682:ARG:NH1	2:B:98:ALA:O	2.21	0.72
1:E:571:ARG:NH2	1:E:595:ASP:O	2.23	0.72
2:F:202:GLU:HG3	2:F:246:MSE:HE1	1.74	0.70
2:B:147:ASN:HB3	2:B:150:HIS:HB2	1.75	0.68
1:E:559:LYS:H	1:E:562:MSE:HE3	1.57	0.67
1:A:571:ARG:NH2	1:A:595:ASP:O	2.27	0.67
1:E:682:ARG:HA	1:E:685:MSE:HE2	1.76	0.66
2:D:127:GLU:O	2:D:131:ASN:ND2	2.29	0.65
1:C:786:SER:O	1:C:790:ASN:ND2	2.29	0.65
1:E:646[B]:ARG:NH1	1:E:648:TYR:OH	2.30	0.64
1:E:469:HIS:NE2	1:E:757:GLU:OE2	2.23	0.64
1:A:682:ARG:NH2	1:A:707:HIS:O	2.31	0.64
1:C:923:ASP:OD1	1:C:924:GLU:N	2.33	0.62
1:E:919:ARG:NH1	2:F:300:ASP:OD2	2.32	0.62
1:C:805:GLN:OE1	1:C:807:ARG:NH1	2.33	0.61
1:E:581:PRO:HB2	1:E:610:ILE:HD11	1.81	0.61
1:A:919:ARG:HG3	2:B:306:VAL:HG12	1.83	0.61
1:E:740:ASP:OD1	1:E:740:ASP:N	2.31	0.60
1:A:776:GLU:OE2	1:A:946:LYS:NZ	2.34	0.60
1:C:503:ARG:O	1:C:506:THR:OG1	2.11	0.60
1:A:786:SER:O	1:A:790:ASN:ND2	2.33	0.59
2:F:266:SER:HB3	2:F:268:PRO:HD2	1.83	0.59
1:A:899:ASN:ND2	2:B:275:ARG:O	2.32	0.59
1:C:584:PRO:O	2:D:179:ARG:NH1	2.35	0.58
1:A:892:MSE:HE3	1:A:895:PRO:HB3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:235:LEU:HD22	2:F:255:ALA:HB2	1.85	0.58
1:A:919:ARG:NH2	2:B:299:GLN:OE1	2.36	0.58
2:D:214:ASP:OD2	2:D:231:LYS:NZ	2.37	0.58
1:C:813:HIS:ND1	1:C:871:GLU:OE2	2.37	0.58
1:C:540:ASP:OD2	2:D:175:LYS:NZ	2.32	0.58
2:D:185:THR:OG1	2:D:186:PHE:N	2.36	0.57
1:A:906:LYS:NZ	1:A:910:ASP:OD1	2.32	0.57
2:D:179:ARG:HH21	4:D:401:TRS:H11	1.69	0.56
1:A:572:LYS:HB3	1:A:577:ASP:HB3	1.87	0.56
1:A:468:GLN:HG2	1:A:526:VAL:HB	1.88	0.56
2:F:105:ASP:OD2	2:F:105:ASP:N	2.34	0.56
1:E:687:ILE:HD13	1:E:724:MSE:HE2	1.86	0.56
1:E:538:ILE:HD11	2:F:185:THR:HG21	1.88	0.55
2:D:205:TYR:HD1	2:D:254:ILE:HG21	1.71	0.55
1:E:574[B]:ASN:OD1	1:E:575:GLU:N	2.39	0.55
1:A:558:SER:O	2:B:184:LYS:NZ	2.40	0.55
1:A:813:HIS:ND1	1:A:871:GLU:OE2	2.40	0.55
1:E:919:ARG:NH2	2:F:299:GLN:OE1	2.39	0.55
2:D:147:ASN:HB3	2:D:150:HIS:HB2	1.89	0.55
1:A:540:ASP:OD2	2:B:175:LYS:NZ	2.40	0.55
1:A:915:LEU:HB3	1:A:935:ILE:HB	1.89	0.55
1:C:571:ARG:NH2	1:C:595:ASP:O	2.40	0.54
1:A:587:GLU:HB2	2:B:180:LYS:HD3	1.90	0.54
1:A:565:LYS:HB3	1:A:567:ILE:HD11	1.88	0.54
2:F:117:ILE:HG12	2:F:188:VAL:HG11	1.88	0.54
1:C:909:ARG:HG3	1:C:938:PRO:HB3	1.89	0.54
2:B:169:THR:HG21	2:B:269:LEU:HD13	1.89	0.54
2:D:294:ASP:OD1	2:D:295:MSE:N	2.41	0.54
1:C:535:ASP:O	2:D:175:LYS:NZ	2.34	0.54
2:B:178:ASP:HB3	2:B:180:LYS:H	1.74	0.53
2:F:221:GLU:HA	2:F:224:GLU:HB3	1.90	0.53
1:A:668:PRO:O	1:A:765:MSE:HG3	2.08	0.53
1:A:892:MSE:HE1	2:B:270:TYR:HB3	1.91	0.53
1:E:936:ARG:HH21	2:F:226:GLU:HB2	1.73	0.53
2:F:207:LEU:O	2:F:257:LYS:NZ	2.32	0.53
2:F:133:LEU:HD23	2:F:138:TYR:HE2	1.74	0.53
1:A:746:ASP:N	1:A:746:ASP:OD1	2.40	0.52
1:C:832:MSE:HA	1:C:864:GLN:HE22	1.75	0.52
1:A:899:ASN:HB2	2:B:274:ASN:O	2.10	0.52
1:A:888:PRO:HB3	1:A:892:MSE:HE2	1.92	0.52
2:D:200:GLU:HB2	2:D:203:GLU:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ARG:NH1	2:B:300:ASP:OD1	2.43	0.52
1:E:796:ILE:HG13	1:E:827:PHE:HB2	1.90	0.51
2:F:178:ASP:OD1	2:F:178:ASP:N	2.42	0.51
1:E:746:ASP:N	1:E:746:ASP:OD2	2.39	0.51
2:F:147:ASN:HB3	2:F:150:HIS:HB2	1.92	0.51
1:E:570:TYR:HD2	1:E:590:VAL:HG13	1.75	0.51
2:F:196:ARG:NH2	2:F:203:GLU:OE1	2.43	0.51
1:A:888:PRO:HB3	1:A:892:MSE:CE	2.41	0.51
1:E:492:HIS:HE1	2:F:287:ASP:OD2	1.93	0.51
1:E:682:ARG:NH2	1:E:707:HIS:O	2.45	0.50
1:A:571:ARG:HD2	1:A:605:VAL:O	2.12	0.50
1:C:888:PRO:HB3	1:C:892:MSE:HE3	1.94	0.50
2:B:167:LEU:HD21	2:B:191:MSE:HE3	1.93	0.50
2:F:143:ILE:HG12	2:F:153:VAL:HG22	1.93	0.50
1:C:516:ARG:NH2	1:C:521:ASP:OD2	2.36	0.49
1:C:675:VAL:HA	1:C:678:MSE:HG3	1.94	0.49
1:E:892:MSE:HE2	1:E:895:PRO:HB3	1.94	0.49
1:E:534:GLN:HB2	1:E:641:PHE:CE2	2.48	0.49
1:E:899:ASN:OD1	1:E:902:ASN:ND2	2.45	0.49
1:E:555:VAL:HB	1:E:619:ILE:HG21	1.95	0.49
1:C:858:SER:OG	1:C:859:TYR:N	2.44	0.49
1:A:899:ASN:O	1:A:903:LYS:HB2	2.13	0.49
1:A:724:MSE:HA	1:A:738:LEU:HA	1.95	0.49
2:B:272:VAL:HG23	2:B:276:ARG:HB3	1.95	0.48
1:E:919:ARG:HG3	2:F:306:VAL:HG12	1.96	0.48
1:A:494:HIS:ND1	2:B:187:ASP:OD2	2.38	0.48
2:D:215:LEU:HD23	2:D:218:LYS:HD3	1.94	0.48
1:A:751:LYS:NZ	2:B:105:ASP:OD1	2.34	0.48
1:E:559:LYS:N	1:E:562:MSE:HE3	2.27	0.48
1:A:897:GLU:HG2	2:B:275:ARG:HG2	1.96	0.48
1:E:776:GLU:HG3	1:E:946:LYS:HE2	1.96	0.48
1:E:548:GLU:HG3	2:F:171:ILE:HG12	1.96	0.48
1:E:565:LYS:NZ	2:F:181:ASN:OD1	2.30	0.48
1:C:935:ILE:HG13	2:D:296:LEU:HD21	1.95	0.47
1:E:476:LEU:HD22	1:E:759:ILE:HD12	1.97	0.47
1:C:520:ARG:O	1:C:520:ARG:NH1	2.43	0.47
1:E:561:GLY:HA2	1:E:562:MSE:O	2.14	0.47
1:C:572:LYS:HB3	1:C:577:ASP:HB3	1.96	0.47
2:F:142:SER:HB3	2:F:154:THR:HB	1.96	0.47
1:E:559:LYS:HG3	1:E:562:MSE:HE3	1.96	0.47
1:A:894:ASN:HB3	1:A:897:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:571:ARG:HD2	1:E:605:VAL:O	2.15	0.47
1:A:510:PHE:CE1	1:A:649:LEU:HB2	2.50	0.47
2:F:250:HIS:ND1	2:F:253:GLU:OE1	2.34	0.47
1:E:559:LYS:NZ	1:E:763:GLU:OE1	2.45	0.46
1:A:469:HIS:NE2	1:A:757:GLU:OE2	2.42	0.46
2:B:209:ALA:O	2:B:212:THR:OG1	2.31	0.46
1:C:559:LYS:NZ	1:C:763:GLU:OE2	2.38	0.46
2:B:105:ASP:OD2	2:B:105:ASP:N	2.49	0.46
2:D:100:ASP:O	2:D:106:ILE:HD11	2.15	0.46
2:B:187:ASP:N	2:B:187:ASP:OD1	2.49	0.46
1:E:729:ASP:HA	1:E:733:LYS:HD2	1.97	0.46
2:D:146:LYS:HD2	2:D:201:GLU:HB3	1.98	0.46
1:A:508:ILE:HB	2:B:143:ILE:HB	1.98	0.45
1:A:639:SER:HB3	1:A:645:ASN:HB3	1.98	0.45
1:E:681:THR:O	1:E:685:MSE:HG3	2.15	0.45
1:C:548:GLU:HG3	2:D:171:ILE:HG12	1.98	0.45
2:B:125:GLN:NE2	2:B:158:VAL:HG21	2.31	0.45
2:D:125:GLN:HG3	2:D:160:TYR:OH	2.16	0.45
1:E:905:VAL:HG21	2:F:219:HIS:CD2	2.52	0.45
1:E:915:LEU:HB3	1:E:935:ILE:HB	1.98	0.45
2:F:147:ASN:ND2	2:F:247:GLU:OE2	2.50	0.45
1:E:684:LYS:HE2	1:E:688:TYR:HE2	1.82	0.45
1:E:601:ASN:N	1:E:601:ASN:OD1	2.49	0.45
1:E:644[B]:SER:OG	1:E:645:ASN:N	2.49	0.45
1:E:547:MSE:HE2	1:E:614:LEU:HD13	1.98	0.45
1:E:771:PHE:HE2	1:E:788:GLU:HG2	1.81	0.45
2:B:314:SER:HA	2:B:315:GLU:HA	1.55	0.45
2:D:221:GLU:HA	2:D:224:GLU:HB3	1.97	0.45
1:E:684:LYS:HE2	1:E:688:TYR:CE2	2.52	0.45
2:B:98:ALA:HB1	2:B:100:ASP:OD2	2.17	0.45
2:F:117:ILE:HG21	2:F:191:MSE:HE2	1.99	0.45
1:C:571:ARG:HD2	1:C:605:VAL:O	2.17	0.45
1:E:546:LEU:HD22	2:F:173:VAL:HG22	1.99	0.45
1:C:465:LEU:HD13	1:C:589[B]:HIS:CE1	2.52	0.44
1:E:516:ARG:NH2	1:E:521:ASP:OD2	2.34	0.44
2:F:185:THR:OG1	2:F:186:PHE:N	2.49	0.44
1:E:791:LEU:HA	1:E:796:ILE:HD13	1.99	0.44
1:C:759:ILE:O	1:C:762:VAL:HG12	2.17	0.44
1:C:951:ASP:HA	1:C:954:ASP:HB2	2.00	0.44
2:B:185:THR:OG1	2:B:186:PHE:N	2.50	0.44
2:B:235:LEU:HD22	2:B:255:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:236:LYS:HB3	2:D:240:GLY:HA2	2.00	0.44
2:B:228:TRP:CD1	2:B:256:LEU:HD22	2.53	0.44
2:F:126:LEU:O	2:F:130:LYS:HG3	2.18	0.43
1:E:520:ARG:NH2	1:E:535:ASP:OD1	2.50	0.43
2:D:117:ILE:HG12	2:D:188:VAL:HG11	2.00	0.43
1:A:721:LYS:O	1:A:739:LYS:NZ	2.31	0.43
2:D:213:GLU:CD	2:D:218:LYS:HD2	2.39	0.43
1:A:710:ASP:OD2	1:A:710:ASP:N	2.44	0.43
1:E:745:LEU:HB2	1:E:749:ALA:HB3	2.00	0.43
1:A:781:ASP:HB3	1:A:784:LEU:HB3	2.00	0.43
2:F:196:ARG:NH1	2:F:197:PRO:O	2.52	0.43
1:E:508:ILE:HB	2:F:143:ILE:HB	2.01	0.43
1:C:796:ILE:HA	1:C:796:ILE:HD13	1.90	0.42
1:A:884:SER:O	1:E:829:LYS:NZ	2.53	0.42
1:E:771:PHE:CE2	1:E:788:GLU:HG2	2.54	0.42
1:E:482:LYS:HE2	2:F:97:GLU:HB3	2.01	0.42
1:A:820:GLY:HA3	1:A:899:ASN:HD21	1.84	0.42
1:A:538:ILE:HD11	2:B:185:THR:HG21	2.02	0.42
1:E:569:TYR:O	1:E:610:ILE:HA	2.19	0.42
1:E:662:PHE:HD1	1:E:800:PHE:CE1	2.38	0.42
1:E:947:ILE:O	1:E:950:GLN:HG2	2.19	0.42
2:B:282:ASP:O	2:B:286:ILE:HG13	2.19	0.42
2:D:98:ALA:HB1	2:D:100:ASP:OD2	2.20	0.42
1:C:631:THR:HB	2:D:120:ILE:O	2.20	0.42
1:A:797:THR:O	1:A:801:ILE:HG12	2.19	0.42
2:B:288:TYR:O	2:B:292:VAL:HG23	2.20	0.42
1:C:555:VAL:HG11	1:C:663:PRO:HB3	2.02	0.42
1:E:780:PHE:HB3	1:E:942:GLN:HG3	2.01	0.42
1:C:495[B]:ARG:NH1	2:D:167:LEU:O	2.52	0.41
1:A:811:GLN:HG2	1:A:830:THR:HB	2.02	0.41
2:D:125:GLN:NE2	2:D:158:VAL:HG21	2.35	0.41
1:C:493:PHE:O	1:C:495[B]:ARG:HG2	2.20	0.41
1:A:894:ASN:HA	1:A:895:PRO:HD2	1.88	0.41
1:E:611:VAL:O	1:E:613:THR:HG23	2.20	0.41
1:E:577:ASP:OD1	1:E:579:LEU:HG	2.20	0.41
1:E:584:PRO:O	2:F:179:ARG:NH1	2.53	0.41
1:E:707:HIS:NE2	2:F:102:GLU:HG2	2.35	0.41
1:A:915:LEU:HB2	1:A:941:ILE:HG12	2.01	0.41
1:C:641:PHE:HA	1:C:641:PHE:HD1	1.75	0.41
1:C:817:ASP:HA	1:C:818:PRO:HD3	1.90	0.41
1:C:706:LYS:HE3	1:C:707:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:TYR:CE2	2:B:176:SER:HB3	2.55	0.41
1:A:858:SER:O	1:A:861:VAL:HG22	2.20	0.41
2:F:271:ASN:O	2:F:275[B]:ARG:HB2	2.21	0.41
1:C:909:ARG:NH2	1:C:911:ASP:OD1	2.51	0.41
1:E:517:LYS:O	1:E:520:ARG:HB3	2.21	0.41
1:A:758:GLN:O	1:A:762:VAL:HG23	2.21	0.41
1:E:619:ILE:HG21	1:E:661:THR:HB	2.02	0.41
1:A:546:LEU:HD22	2:B:173:VAL:HG22	2.02	0.41
1:E:888:PRO:O	1:E:892:MSE:HB2	2.20	0.40
1:E:564:ASN:OD1	1:E:616:ASN:ND2	2.53	0.40
1:C:864:GLN:HE21	1:C:864:GLN:HB3	1.75	0.40
1:C:495[B]:ARG:HB3	1:C:495[B]:ARG:HE	1.69	0.40
2:B:178:ASP:O	2:B:179:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	469/506 (93%)	449 (96%)	18 (4%)	2 (0%)	39 74
1	C	454/506 (90%)	433 (95%)	21 (5%)	0	100 100
1	E	472/506 (93%)	451 (96%)	20 (4%)	1 (0%)	52 84
2	B	227/235 (97%)	220 (97%)	7 (3%)	0	100 100
2	D	224/235 (95%)	216 (96%)	8 (4%)	0	100 100
2	F	226/235 (96%)	212 (94%)	14 (6%)	0	100 100
All	All	2072/2223 (93%)	1981 (96%)	88 (4%)	3 (0%)	56 87

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	685	MSE
1	E	561	GLY
1	A	812	ILE

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	396/449 (88%)	374 (94%)	22 (6%)	26	60
1	C	360/449 (80%)	345 (96%)	15 (4%)	36	73
1	E	414/449 (92%)	385 (93%)	29 (7%)	19	47
2	B	200/209 (96%)	191 (96%)	9 (4%)	34	70
2	D	190/209 (91%)	182 (96%)	8 (4%)	36	73
2	F	201/209 (96%)	193 (96%)	8 (4%)	38	74
All	All	1761/1974 (89%)	1670 (95%)	91 (5%)	29	64

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	SER
1	A	483	VAL
1	A	520	ARG
1	A	636	THR
1	A	685	MSE
1	A	710	ASP
1	A	722	GLU
1	A	746	ASP
1	A	750	VAL
1	A	765	MSE
1	A	782	SER
1	A	804	THR
1	A	821	CYS
1	A	857	HIS
1	A	875	THR
1	A	886	SER

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Mol	Chain	Res	Type
1	A	911	ASP
1	A	918	VAL
1	A	932	THR
1	A	933	ILE
1	A	953	GLU
1	A	954	ASP
1	C	465	LEU
1	C	477	GLN
1	C	478	SER
1	C	485	VAL
1	C	522	LYS
1	C	636	THR
1	C	695	HIS
1	C	706	LYS
1	C	744	LEU
1	C	762	VAL
1	C	821	CYS
1	C	830	THR
1	C	832	MSE
1	C	911	ASP
1	C	953	GLU
1	E	478	SER
1	E	482	LYS
1	E	541	THR
1	E	577	ASP
1	E	578	THR
1	E	587	GLU
1	E	589[A]	HIS
1	E	589[B]	HIS
1	E	593	VAL
1	E	601	ASN
1	E	606	GLU
1	E	628	ILE
1	E	646[A]	ARG
1	E	646[B]	ARG
1	E	704	ILE
1	E	715	GLN
1	E	718	GLN
1	E	740	ASP
1	E	745	LEU
1	E	746	ASP
1	E	767	GLN

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Mol	Chain	Res	Type
1	E	773	GLU
1	E	788	GLU
1	E	796	ILE
1	E	821	CYS
1	E	860	ASN
1	E	866	LYS
1	E	892	MSE
1	E	919	ARG
2	B	90	LYS
2	B	97	GLU
2	B	105	ASP
2	B	170	VAL
2	B	178	ASP
2	B	187	ASP
2	B	221	GLU
2	B	229	GLU
2	B	295	MSE
2	D	105	ASP
2	D	112	ILE
2	D	154	THR
2	D	177	VAL
2	D	179	ARG
2	D	280	LYS
2	D	287	ASP
2	D	314	SER
2	F	104	SER
2	F	105	ASP
2	F	108	ASP
2	F	158	VAL
2	F	221	GLU
2	F	254	ILE
2	F	307	SER
2	F	309	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	492	HIS

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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	TRS	D	401	-	7,7,7	0.93	1 (14%)	9,9,9	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	D	401	-	-	0/9/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	TRS	C-N	-2.42	1.47	1.50

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	TRS	1	0

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	459/506 (90%)	0.05	2 (0%) 93 92	54, 76, 120, 153	0
1	C	449/506 (88%)	0.40	31 (6%) 20 14	43, 84, 163, 191	0
1	E	457/506 (90%)	0.20	4 (0%) 85 84	44, 70, 102, 133	0
2	B	224/235 (95%)	0.08	0 100 100	52, 73, 103, 149	0
2	D	220/235 (93%)	0.32	7 (3%) 51 43	50, 86, 131, 141	0
2	F	220/235 (93%)	0.15	1 (0%) 91 90	49, 76, 110, 131	0
All	All	2029/2223 (91%)	0.21	45 (2%) 65 60	43, 77, 128, 191	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	694	ASN	4.9
2	D	307	SER	4.7
1	C	691	LEU	4.2
1	C	703	PRO	4.0
1	C	693	HIS	3.9
1	C	704	ILE	3.9
1	C	695	HIS	3.8
1	C	775	ASN	3.6
1	C	696	SER	3.5
2	D	99	TYR	3.3
1	E	462	ILE	3.2
1	C	701	ILE	3.2
2	D	102	GLU	3.1
2	D	308	TYR	2.9
1	C	725	LYS	2.9
1	C	708	PHE	2.8
1	C	510	PHE	2.8
1	C	719	LYS	2.7
2	D	101	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	702	ASP	2.6
1	C	944	TYR	2.6
1	E	649	LEU	2.5
1	C	916	LYS	2.5
1	C	706	LYS	2.4
1	A	859	TYR	2.4
1	C	861	VAL	2.4
1	C	792	LEU	2.4
1	C	935	ILE	2.4
1	E	610	ILE	2.4
1	C	700	SER	2.4
1	C	738	LEU	2.4
1	C	499	GLY	2.3
1	C	480	PHE	2.3
1	C	741	ASP	2.2
1	C	915	LEU	2.2
2	D	242	PRO	2.2
1	C	726	TYR	2.2
2	F	146	LYS	2.2
1	C	705	ALA	2.2
1	C	918	VAL	2.2
1	A	831	SER	2.1
2	D	98	ALA	2.1
1	C	688	TYR	2.0
1	E	651	ASN	2.0
1	C	642	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	A	1001	1/1	0.77	0.08	-4.26	134,134,134,134	0
4	TRS	D	401	8/8	0.85	0.16	-	97,103,107,108	0

6.5 Other polymers (i)

There are no such residues in this entry.