Full wwPDB X-ray Structure Validation Report (i)

Oct 28, 2024 – 02:26 PM EDT

PDB ID	:	8TX8
Title	:	Crystal Structure of RBBP4 bound to ZNF512B peptide
Authors	:	Deshpande, C.N.; Mackay, J.P.
Deposited on	:	2023-08-22
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

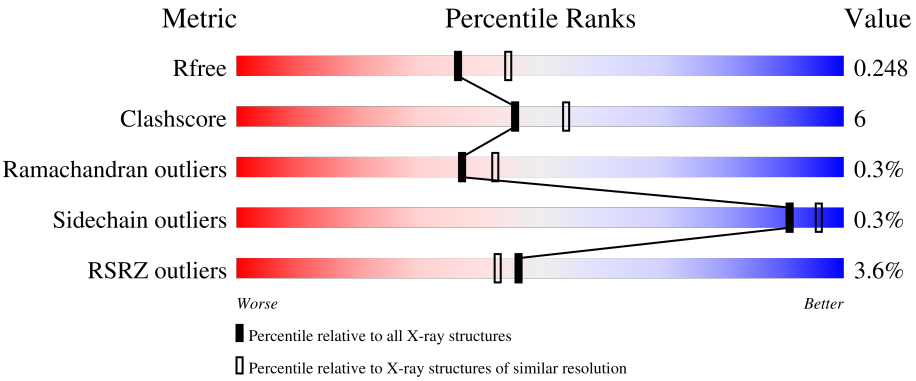
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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 <=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	445	4% 71% 13% 16%
1	B	445	2% 72% 12% 16%
2	C	13	92% 8%
2	D	13	85% 15%

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	FMT	A	1001	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6600 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 Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2982	1885	510	577	10			
1	B	373	Total	C	N	O	S	0	0	0
			2981	1884	511	576	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q09028
A	-18	GLY	-	expression tag	UNP Q09028
A	-17	SER	-	expression tag	UNP Q09028
A	-16	SER	-	expression tag	UNP Q09028
A	-15	HIS	-	expression tag	UNP Q09028
A	-14	HIS	-	expression tag	UNP Q09028
A	-13	HIS	-	expression tag	UNP Q09028
A	-12	HIS	-	expression tag	UNP Q09028
A	-11	HIS	-	expression tag	UNP Q09028
A	-10	HIS	-	expression tag	UNP Q09028
A	-9	SER	-	expression tag	UNP Q09028
A	-8	SER	-	expression tag	UNP Q09028
A	-7	GLY	-	expression tag	UNP Q09028
A	-6	LEU	-	expression tag	UNP Q09028
A	-5	VAL	-	expression tag	UNP Q09028
A	-4	PRO	-	expression tag	UNP Q09028
A	-3	ARG	-	expression tag	UNP Q09028
A	-2	GLY	-	expression tag	UNP Q09028
A	-1	SER	-	expression tag	UNP Q09028
A	0	HIS	-	expression tag	UNP Q09028
B	-19	MET	-	initiating methionine	UNP Q09028
B	-18	GLY	-	expression tag	UNP Q09028
B	-17	SER	-	expression tag	UNP Q09028
B	-16	SER	-	expression tag	UNP Q09028
B	-15	HIS	-	expression tag	UNP Q09028

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q09028
B	-13	HIS	-	expression tag	UNP Q09028
B	-12	HIS	-	expression tag	UNP Q09028
B	-11	HIS	-	expression tag	UNP Q09028
B	-10	HIS	-	expression tag	UNP Q09028
B	-9	SER	-	expression tag	UNP Q09028
B	-8	SER	-	expression tag	UNP Q09028
B	-7	GLY	-	expression tag	UNP Q09028
B	-6	LEU	-	expression tag	UNP Q09028
B	-5	VAL	-	expression tag	UNP Q09028
B	-4	PRO	-	expression tag	UNP Q09028
B	-3	ARG	-	expression tag	UNP Q09028
B	-2	GLY	-	expression tag	UNP Q09028
B	-1	SER	-	expression tag	UNP Q09028
B	0	HIS	-	expression tag	UNP Q09028

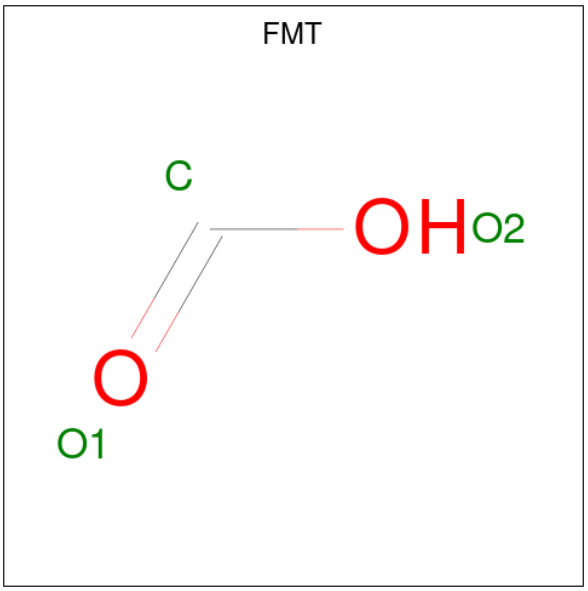
- Molecule 2 is a protein called Zinc finger protein 512B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	0	0	0
			114	73	26	15			
2	D	13	Total	C	N	O	0	0	0
			114	73	26	15			

There are 2 discrepancies between the modelled and reference sequences:

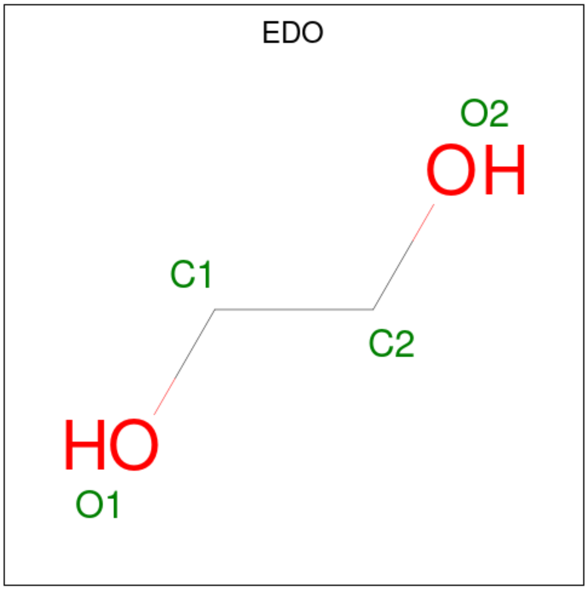
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ACE	-	expression tag	UNP Q96KM6
D	0	ACE	-	expression tag	UNP Q96KM6

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



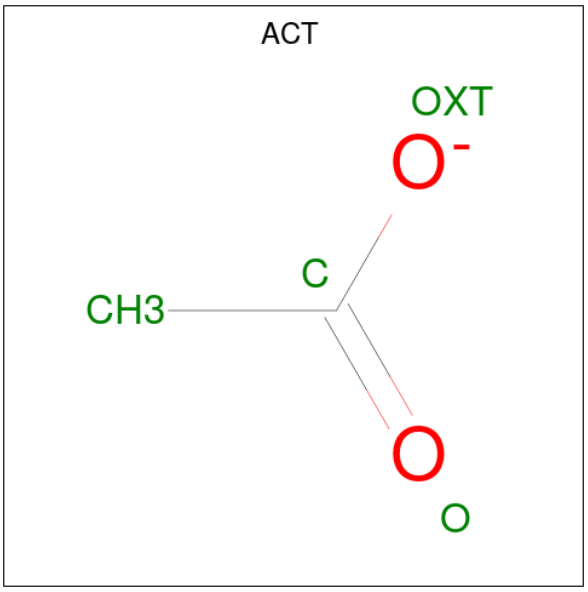
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



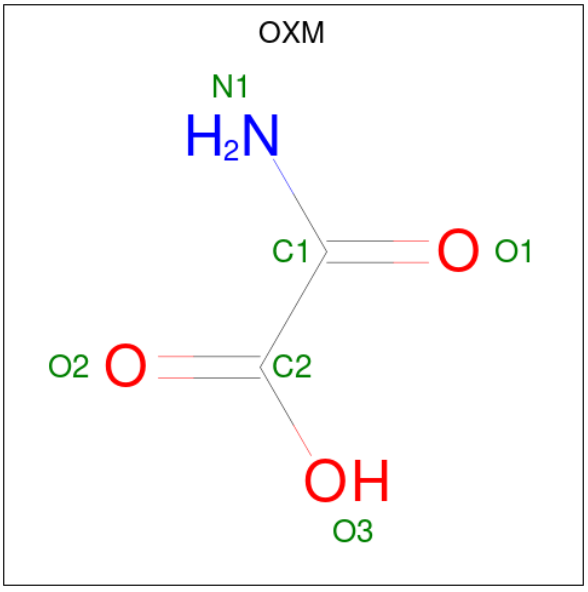
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 7 is water.

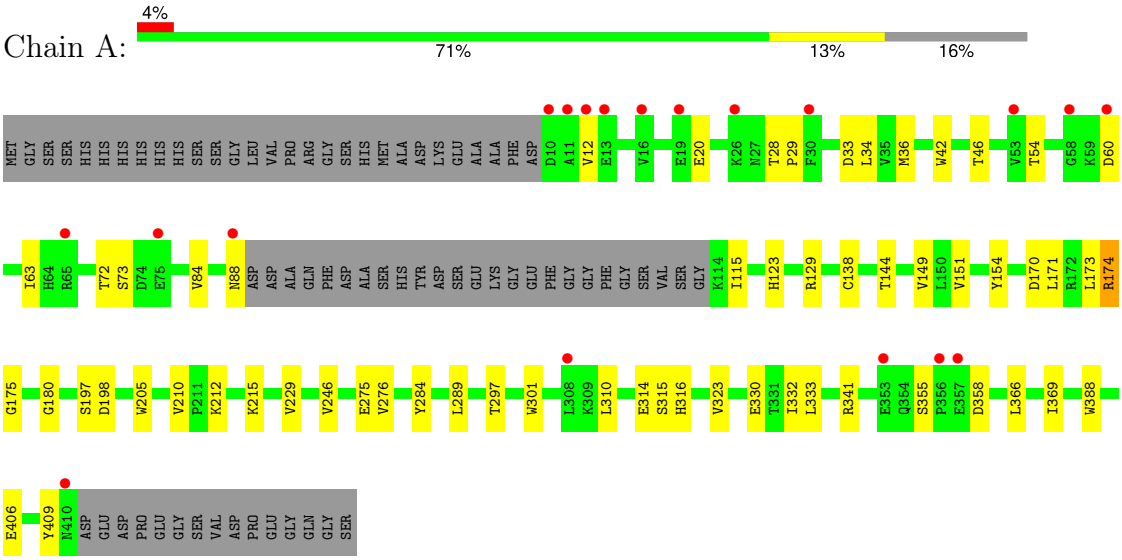
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	170	Total O 170 170	0	0
7	B	153	Total O 153 153	0	0
7	C	2	Total O 2 2	0	0
7	D	12	Total O 12 12	0	0

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.

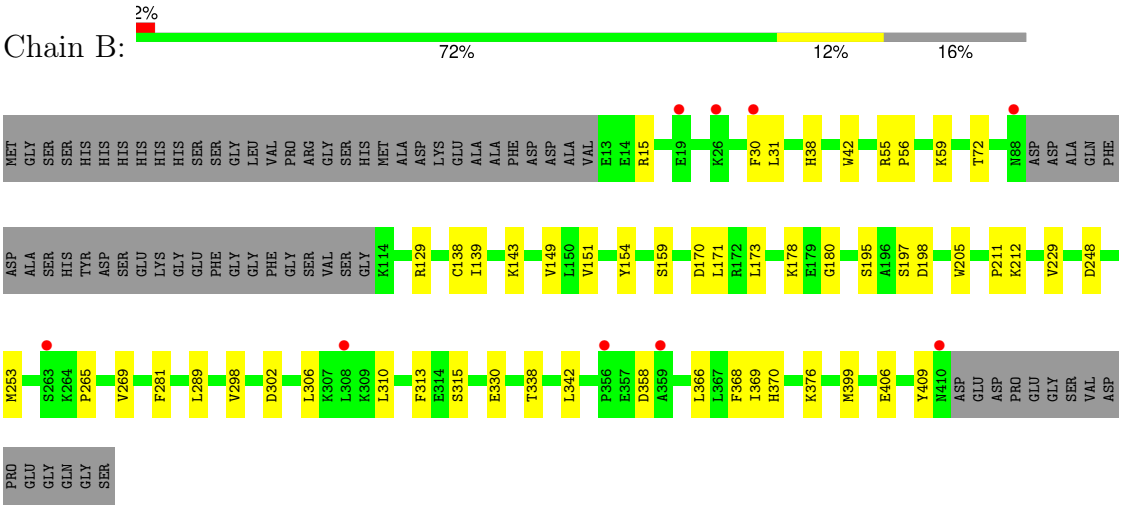
• Molecule 1: Histone-binding protein RBBP4

Chain A:



• Molecule 1: Histone-binding protein RBBP4

Chain B:

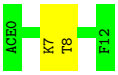


• Molecule 2: Zinc finger protein 512B

Chain C:

• Molecule 2: Zinc finger protein 512B

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.10Å 59.58Å 101.45Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	46.88 – 2.20 46.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.88-2.20) 99.9 (46.88-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.208 , 0.244 0.214 , 0.248	Depositor DCC
R_{free} test set	2386 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6600	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.38% 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: ACT, ACE, FMT, OXM, EDO

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	0.32	0/3065	0.56	2/4183 (0.0%)
1	B	0.28	0/3064	0.51	0/4178
2	C	0.28	0/114	0.57	0/147
2	D	0.37	0/114	0.62	0/147
All	All	0.30	0/6357	0.54	2/8655 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	VAL	N-CA-C	-8.40	88.33	111.00
1	A	316	HIS	N-CA-C	-6.61	93.16	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	ARG	Sidechain
1	B	129	ARG	Sidechain

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	2982	0	2835	38	1
1	B	2981	0	2852	33	1
2	C	114	0	132	1	0
2	D	114	0	132	1	0
3	A	6	0	2	2	0
3	B	6	0	2	1	0
3	C	3	0	1	0	0
3	D	3	0	1	0	0
4	A	28	0	42	2	0
4	B	16	0	24	2	0
5	B	4	0	3	0	0
6	B	6	0	2	1	0
7	A	170	0	0	0	0
7	B	153	0	0	0	0
7	C	2	0	0	0	0
7	D	12	0	0	0	0
All	All	6600	0	6028	70	1

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 (70) 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:B:253:MET:HG2	1:B:265:PRO:HG3	1.47	0.96
1:A:174:ARG:HH22	3:A:1001:FMT:H	1.42	0.83
2:D:7:LYS:HG2	2:D:8:THR:HG23	1.68	0.76
1:B:302:ASP:HB2	1:B:310:LEU:HD11	1.76	0.67
1:B:269:VAL:HG21	1:B:306:LEU:HB3	1.80	0.64
1:A:151:VAL:HB	1:A:171:LEU:HB2	1.80	0.63
1:B:151:VAL:HB	1:B:171:LEU:HB2	1.81	0.61
1:A:210:VAL:HG13	1:A:215:LYS:HD3	1.83	0.61
1:B:298:VAL:HB	1:B:313:PHE:HB2	1.85	0.59
1:B:330:GLU:HB3	6:B:502:OXM:HN1	1.67	0.59
1:B:149:VAL:HB	1:B:173:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:HD12	1:B:212:LYS:HE2	1.87	0.55
1:A:323:VAL:HG22	1:A:333:LEU:HD11	1.88	0.55
1:A:173:LEU:HB3	1:A:205:TRP:CE2	2.43	0.54
1:B:143:LYS:NZ	1:B:195:SER:OG	2.33	0.54
1:A:54:THR:HG23	1:A:63:ILE:HB	1.91	0.53
1:A:330:GLU:H	1:A:330:GLU:CD	2.12	0.53
1:B:281:PHE:CE1	1:B:289:LEU:HD23	2.44	0.53
1:A:289:LEU:C	1:A:289:LEU:HD12	2.30	0.52
1:B:56:PRO:HB2	1:B:59:LYS:HD2	1.92	0.52
1:A:42:TRP:CG	1:A:72:THR:HG22	2.47	0.50
1:A:34:LEU:HD21	1:A:36:MET:HE3	1.94	0.50
1:A:366:LEU:HD21	1:A:369:ILE:HD11	1.93	0.50
1:B:38:HIS:HB3	1:B:399:MET:HE3	1.93	0.50
1:B:180:GLY:HA3	1:B:197:SER:HA	1.94	0.48
1:A:174:ARG:NH2	3:A:1001:FMT:H	2.19	0.48
1:B:229:VAL:H	4:B:503:EDO:H12	1.77	0.48
1:A:174:ARG:HG3	1:A:175:GLY:N	2.27	0.48
1:B:173:LEU:HB3	1:B:205:TRP:CE2	2.49	0.48
1:A:149:VAL:HB	1:A:173:LEU:HB2	1.95	0.48
1:A:28:THR:OG1	1:A:29:PRO:HD3	2.13	0.47
1:B:366:LEU:HD21	1:B:369:ILE:HD11	1.97	0.47
1:B:170:ASP:HB3	1:B:212:LYS:HB3	1.96	0.47
1:B:55:ARG:O	4:B:505:EDO:H12	2.15	0.46
1:B:406:GLU:HA	1:B:409:TYR:CZ	2.51	0.46
1:A:46:THR:HB	1:A:129:ARG:HA	1.98	0.46
1:A:284:TYR:HB2	1:A:330:GLU:HB3	1.98	0.46
1:A:355:SER:HB3	1:A:358:ASP:HB2	1.98	0.45
1:B:289:LEU:HD12	1:B:289:LEU:C	2.36	0.45
1:B:42:TRP:CG	1:B:72:THR:HG22	2.51	0.45
1:B:31:LEU:HB3	1:B:368:PHE:HE1	1.81	0.45
1:A:170:ASP:HB3	1:A:212:LYS:HB3	1.98	0.45
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.84	0.45
1:B:138:CYS:HA	1:B:154:TYR:CE2	2.52	0.45
1:B:342:LEU:HB3	1:B:370:HIS:HB3	1.97	0.45
1:A:138:CYS:HA	1:A:154:TYR:CE2	2.52	0.44
1:B:178:LYS:NZ	3:B:506:FMT:H	2.33	0.44
1:A:198:ASP:HA	1:A:229:VAL:HG13	1.99	0.44
1:B:197:SER:OG	1:B:198:ASP:N	2.49	0.44
1:A:123:HIS:CE1	1:A:144:THR:HG22	2.53	0.44
1:A:20:GLU:OE1	1:A:341:ARG:NH2	2.51	0.43
1:A:406:GLU:HA	1:A:409:TYR:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:CE1	1:B:289:LEU:CD2	3.01	0.43
1:A:289:LEU:CD1	1:A:301:TRP:HB2	2.49	0.43
1:A:28:THR:N	1:A:29:PRO:CD	2.82	0.43
1:A:60:ASP:O	1:A:88:ASN:N	2.51	0.43
1:A:84:VAL:HG22	1:A:115:ILE:HG12	2.01	0.43
1:B:269:VAL:CG2	1:B:306:LEU:HB3	2.48	0.42
1:A:310:LEU:HD11	4:A:1003:EDO:H22	2.01	0.42
1:A:210:VAL:CG1	1:A:215:LYS:HD3	2.46	0.42
1:B:248:ASP:OD1	2:C:1:LYS:HE3	2.20	0.42
1:A:180:GLY:HA3	1:A:197:SER:HA	2.02	0.41
1:B:338:THR:HA	1:B:376:LYS:HG2	2.02	0.41
1:A:297:THR:HG22	1:A:314:GLU:HG2	2.02	0.41
1:A:275:GLU:HG3	4:A:1004:EDO:H12	2.03	0.41
1:A:246:VAL:HB	1:A:276:VAL:HB	2.03	0.41
1:A:73:SER:OG	1:B:211:PRO:HA	2.21	0.41
1:A:73:SER:OG	1:B:211:PRO:HB3	2.21	0.40
1:A:332:ILE:HG13	1:A:388:TRP:CH2	2.56	0.40
1:B:30:PHE:CD1	1:B:30:PHE:N	2.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASP:OD1	1:B:15:ARG:NH2[1_445]	1.62	0.58

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	372/445 (84%)	359 (96%)	12 (3%)	1 (0%)	37	42
1	B	369/445 (83%)	360 (98%)	8 (2%)	1 (0%)	37	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	11/13 (85%)	11 (100%)	0	0	100 100
2	D	11/13 (85%)	11 (100%)	0	0	100 100
All	All	763/916 (83%)	741 (97%)	20 (3%)	2 (0%)	37 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	SER
1	B	315	SER

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	333/392 (85%)	333 (100%)	0	100 100
1	B	336/392 (86%)	334 (99%)	2 (1%)	84 91
2	C	12/12 (100%)	12 (100%)	0	100 100
2	D	12/12 (100%)	12 (100%)	0	100 100
All	All	693/808 (86%)	691 (100%)	2 (0%)	91 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	159	SER
1	B	358	ASP

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

Mol	Chain	Res	Type
1	A	324	GLN
1	A	354	GLN
1	B	410	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

19 ligands are 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	FMT	D	701	-	2,2,2	0.72	0	1,1,1	0.22	0
6	OXM	B	502	-	5,5,5	2.92	1 (20%)	2,6,6	0.49	0
4	EDO	A	1005	-	3,3,3	0.42	0	2,2,2	0.38	0
3	FMT	A	1006	-	2,2,2	0.72	0	1,1,1	0.20	0
4	EDO	A	1009	-	3,3,3	0.45	0	2,2,2	0.29	0
4	EDO	A	1003	-	3,3,3	0.42	0	2,2,2	0.40	0
4	EDO	A	1002	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	B	503	-	3,3,3	0.41	0	2,2,2	0.42	0
4	EDO	B	507	-	3,3,3	0.44	0	2,2,2	0.29	0
3	FMT	B	508	-	2,2,2	0.72	0	1,1,1	0.22	0
5	ACT	B	501	-	3,3,3	1.39	0	3,3,3	1.51	0
4	EDO	B	504	-	3,3,3	0.45	0	2,2,2	0.32	0
3	FMT	C	101	-	2,2,2	0.70	0	1,1,1	0.23	0
4	EDO	A	1007	-	3,3,3	0.44	0	2,2,2	0.40	0
3	FMT	B	506	-	2,2,2	0.72	0	1,1,1	0.23	0
4	EDO	A	1008	-	3,3,3	0.44	0	2,2,2	0.35	0
3	FMT	A	1001	-	2,2,2	0.90	0	1,1,1	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	A	1004	-	3,3,3	0.43	0	2,2,2	0.40	0
4	EDO	B	505	-	3,3,3	0.42	0	2,2,2	0.36	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
6	OXM	B	502	-	-	4/4/4/4	-
4	EDO	A	1007	-	-	0/1/1/1	-
4	EDO	A	1005	-	-	0/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	A	1008	-	-	0/1/1/1	-
4	EDO	A	1004	-	-	0/1/1/1	-
4	EDO	A	1009	-	-	1/1/1/1	-
4	EDO	A	1003	-	-	0/1/1/1	-
4	EDO	A	1002	-	-	0/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	OXM	C1-C2	-6.11	1.48	1.55

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	502	OXM	N1-C1-C2-O2
6	B	502	OXM	N1-C1-C2-O3
6	B	502	OXM	O1-C1-C2-O2
6	B	502	OXM	O1-C1-C2-O3
4	A	1009	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	502	OXM	1	0
4	A	1003	EDO	1	0
4	B	503	EDO	1	0
3	B	506	FMT	1	0
3	A	1001	FMT	2	0
4	A	1004	EDO	1	0
4	B	505	EDO	1	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

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	376/445 (84%)	0.09	19 (5%) 34 31	24, 36, 70, 116	0
1	B	373/445 (83%)	0.10	9 (2%) 59 56	27, 38, 68, 101	0
2	C	12/13 (92%)	0.34	0 100 100	37, 43, 51, 53	0
2	D	12/13 (92%)	0.12	0 100 100	34, 42, 50, 53	0
All	All	773/916 (84%)	0.10	28 (3%) 46 43	24, 37, 69, 116	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	ALA	4.9
1	A	19	GLU	4.1
1	B	30	PHE	4.0
1	A	10	ASP	3.8
1	B	410	ASN	3.7
1	A	26	LYS	3.7
1	A	75	GLU	3.7
1	A	410	ASN	3.5
1	A	353	GLU	3.3
1	A	12	VAL	3.2
1	B	26	LYS	3.2
1	A	308	LEU	3.1
1	B	88	ASN	3.1
1	B	356	PRO	2.9
1	A	65	ARG	2.6
1	B	359	ALA	2.5
1	A	13	GLU	2.4
1	A	356	PRO	2.4
1	B	263	SER	2.4
1	A	88	ASN	2.4
1	A	30	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	357	GLU	2.3
1	B	308	LEU	2.2
1	A	58	GLY	2.2
1	A	16	VAL	2.1
1	A	53	VAL	2.1
1	B	19	GLU	2.1
1	A	60	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no 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	FMT	A	1006	3/3	0.65	0.24	58,58,63,63	0
4	EDO	B	507	4/4	0.65	0.19	52,59,65,66	0
4	EDO	B	505	4/4	0.73	0.22	54,54,57,64	0
4	EDO	A	1002	4/4	0.77	0.15	54,54,63,65	0
6	OXM	B	502	6/6	0.77	0.14	68,73,79,81	0
3	FMT	B	506	3/3	0.80	0.13	51,51,56,58	0
4	EDO	A	1008	4/4	0.81	0.13	62,64,68,69	0
3	FMT	A	1001	3/3	0.81	0.17	48,48,49,52	0
4	EDO	B	503	4/4	0.82	0.23	42,43,43,53	0
4	EDO	A	1005	4/4	0.82	0.23	57,60,62,71	0
5	ACT	B	501	4/4	0.84	0.16	41,42,51,56	0
4	EDO	B	504	4/4	0.85	0.12	40,44,44,46	0
4	EDO	A	1003	4/4	0.86	0.20	41,45,53,60	0
3	FMT	B	508	3/3	0.89	0.12	49,49,52,55	0
4	EDO	A	1009	4/4	0.89	0.18	41,48,52,57	0
3	FMT	C	101	3/3	0.90	0.10	31,31,35,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	1007	4/4	0.90	0.10	44,48,48,50	0
3	FMT	D	701	3/3	0.91	0.12	38,38,43,45	0
4	EDO	A	1004	4/4	0.91	0.16	45,49,51,55	0

6.5 Other polymers (i)

There are no such residues in this entry.