Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2024 – 01:09 PM EDT

PDB ID	:	3VEP
Title	:	Crystal structure of SigD4 in complex with its negative regulator RsdA
Authors	:	Jaiswal, R.K.; Gopal, B.
Deposited on	:	2012-01-09
Resolution	:	2.50 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:

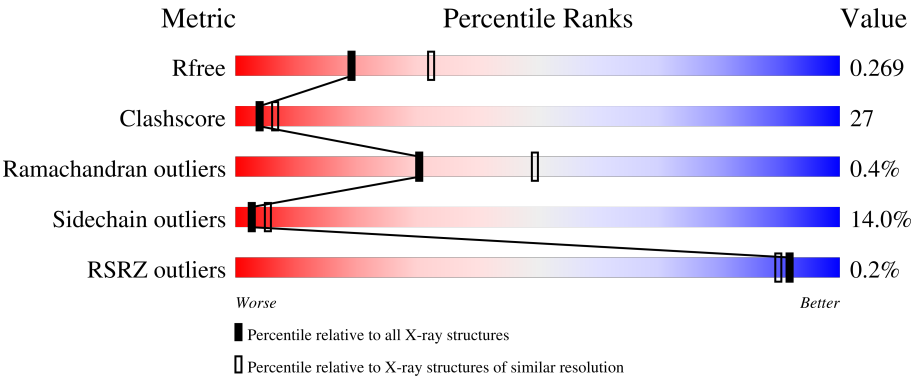
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.50 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	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	C	80	41% 14% • 41%
1	G	80	39% 15% 5% 41%
1	J	80	41% 11% 5% • 41%
1	X	80	44% 10% • 42%
2	A	86	55% 19% 8% 19%

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Mol	Chain	Length	Quality of chain
2	D	86	44% 28% 7% 21%
2	E	86	% 45% 29% 7% 19%
2	H	86	50% 26% 7% 17%

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	E	302	-	-	X	-
3	SO4	E	303	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3680 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 Uncharacterized protein Rv3413c/MT3522.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	X	46	Total	C	N	O	0	0	0
			372	234	64	74			
1	C	47	Total	C	N	O	0	0	0
			379	239	65	75			
1	G	47	Total	C	N	O	0	0	0
			377	237	65	75			
1	J	47	Total	C	N	O	0	0	0
			376	236	65	75			

- Molecule 2 is a protein called Probable RNA polymerase sigma-D factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	68	Total	C	N	O	Se	0	0	0
			505	313	93	97	2			
2	A	70	Total	C	N	O	Se	0	0	0
			511	316	92	101	2			
2	E	70	Total	C	N	O	Se	0	0	0
			517	319	95	101	2			
2	H	71	Total	C	N	O	Se	0	0	0
			526	325	97	102	2			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	127	MSE	-	expression tag	UNP P66811
D	128	GLY	-	expression tag	UNP P66811
D	129	SER	-	expression tag	UNP P66811
D	130	SER	-	expression tag	UNP P66811
D	131	HIS	-	expression tag	UNP P66811
D	132	HIS	-	expression tag	UNP P66811
D	133	HIS	-	expression tag	UNP P66811
D	134	HIS	-	expression tag	UNP P66811

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Chain	Residue	Modelled	Actual	Comment	Reference
D	135	HIS	-	expression tag	UNP P66811
D	136	HIS	-	expression tag	UNP P66811
D	137	SER	-	expression tag	UNP P66811
D	138	GLN	-	expression tag	UNP P66811
D	139	ASP	-	expression tag	UNP P66811
D	140	PRO	-	expression tag	UNP P66811
A	127	MSE	-	expression tag	UNP P66811
A	128	GLY	-	expression tag	UNP P66811
A	129	SER	-	expression tag	UNP P66811
A	130	SER	-	expression tag	UNP P66811
A	131	HIS	-	expression tag	UNP P66811
A	132	HIS	-	expression tag	UNP P66811
A	133	HIS	-	expression tag	UNP P66811
A	134	HIS	-	expression tag	UNP P66811
A	135	HIS	-	expression tag	UNP P66811
A	136	HIS	-	expression tag	UNP P66811
A	137	SER	-	expression tag	UNP P66811
A	138	GLN	-	expression tag	UNP P66811
A	139	ASP	-	expression tag	UNP P66811
A	140	PRO	-	expression tag	UNP P66811
E	127	MSE	-	expression tag	UNP P66811
E	128	GLY	-	expression tag	UNP P66811
E	129	SER	-	expression tag	UNP P66811
E	130	SER	-	expression tag	UNP P66811
E	131	HIS	-	expression tag	UNP P66811
E	132	HIS	-	expression tag	UNP P66811
E	133	HIS	-	expression tag	UNP P66811
E	134	HIS	-	expression tag	UNP P66811
E	135	HIS	-	expression tag	UNP P66811
E	136	HIS	-	expression tag	UNP P66811
E	137	SER	-	expression tag	UNP P66811
E	138	GLN	-	expression tag	UNP P66811
E	139	ASP	-	expression tag	UNP P66811
E	140	PRO	-	expression tag	UNP P66811
H	127	MSE	-	expression tag	UNP P66811
H	128	GLY	-	expression tag	UNP P66811
H	129	SER	-	expression tag	UNP P66811
H	130	SER	-	expression tag	UNP P66811
H	131	HIS	-	expression tag	UNP P66811
H	132	HIS	-	expression tag	UNP P66811
H	133	HIS	-	expression tag	UNP P66811
H	134	HIS	-	expression tag	UNP P66811

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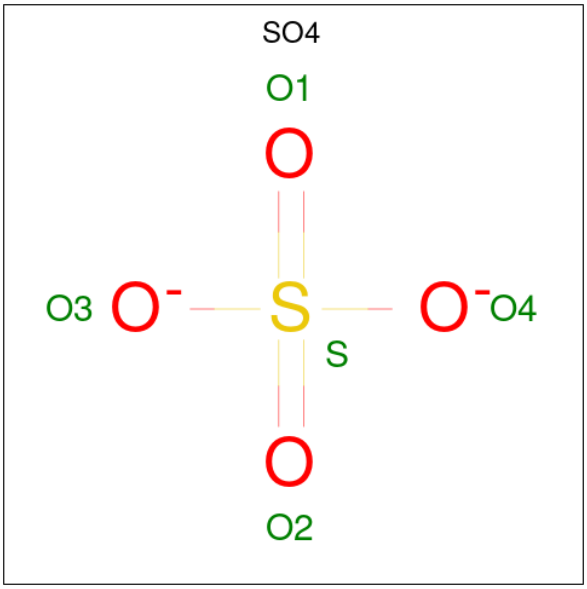
Chain	Residue	Modelled	Actual	Comment	Reference
H	135	HIS	-	expression tag	UNP P66811
H	136	HIS	-	expression tag	UNP P66811
H	137	SER	-	expression tag	UNP P66811
H	138	GLN	-	expression tag	UNP P66811
H	139	ASP	-	expression tag	UNP P66811
H	140	PRO	-	expression tag	UNP P66811

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	X	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

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

- Molecule 4 is water.

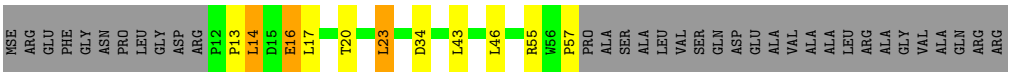
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	X	5	Total O 5 5	0	0
4	D	6	Total O 6 6	0	0
4	C	9	Total O 9 9	0	0
4	A	10	Total O 10 10	0	0
4	G	6	Total O 6 6	0	0
4	E	3	Total O 3 3	0	0
4	J	6	Total O 6 6	0	0
4	H	7	Total O 7 7	0	0

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.

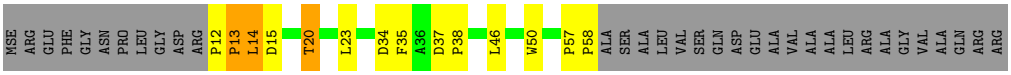
• Molecule 1: Uncharacterized protein Rv3413c/MT3522

Chain X:



• Molecule 1: Uncharacterized protein Rv3413c/MT3522

Chain C:

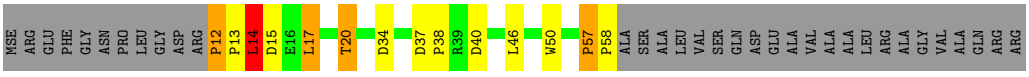


• Molecule 1: Uncharacterized protein Rv3413c/MT3522

Chain G:

• Molecule 1: Uncharacterized protein Rv3413c/MT3522

Chain J:

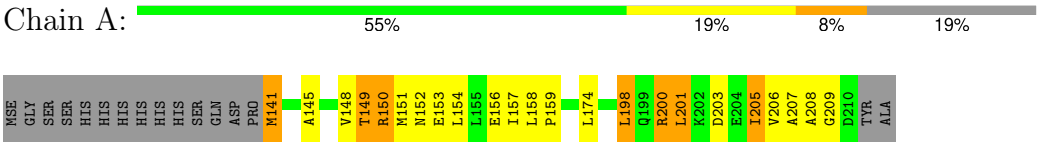


• Molecule 2: Probable RNA polymerase sigma-D factor

Chain D:

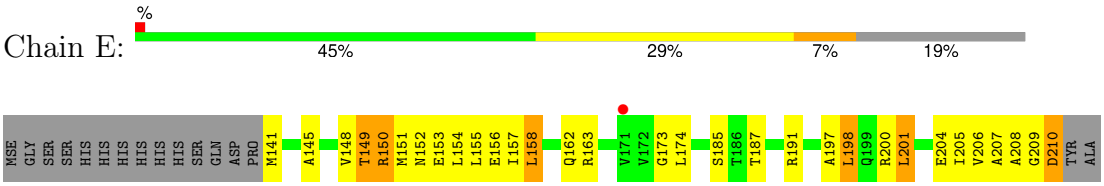
• Molecule 2: Probable RNA polymerase sigma-D factor

Chain A:



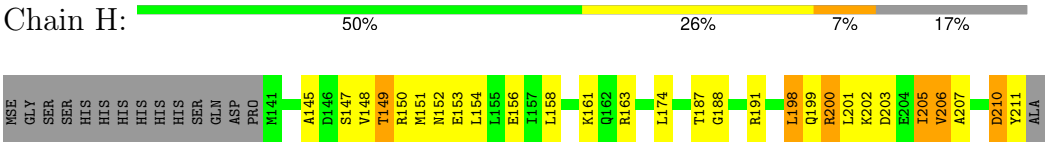
• Molecule 2: Probable RNA polymerase sigma-D factor

Chain E:



• Molecule 2: Probable RNA polymerase sigma-D factor

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.74Å 110.72Å 73.13Å 90.00° 133.00° 90.00°	Depositor
Resolution (Å)	38.47 – 2.50 38.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.6 (38.47-2.50) 86.4 (38.47-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.243 , 0.287 0.252 , 0.269	Depositor DCC
R_{free} test set	900 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-h-2*l,1/2*h-1/2*k 0.017 for -h,h+2*l,1/2*h+1/2*k 0.428 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3680	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% 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: 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	C	0.50	0/388	0.86	0/531
1	G	0.55	0/385	0.87	0/527
1	J	0.47	0/385	0.76	1/527 (0.2%)
1	X	0.56	0/380	0.77	0/519
2	A	0.56	0/511	0.72	1/691 (0.1%)
2	D	0.61	0/505	0.84	3/682 (0.4%)
2	E	0.57	1/517 (0.2%)	0.71	1/698 (0.1%)
2	H	0.57	0/526	0.79	1/709 (0.1%)
All	All	0.55	1/3597 (0.0%)	0.79	7/4884 (0.1%)

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	J	0	1
2	A	0	2
2	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	141	MSE	CG-SE	-5.02	1.78	1.95

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	12	PRO	C-N-CD	-8.30	102.34	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	150	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	D	183	VAL	CG1-CB-CG2	5.55	119.78	110.90
2	H	163	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	D	150	ARG	CB-CG-CD	-5.13	98.27	111.60
2	A	150	ARG	CB-CG-CD	-5.03	98.52	111.60
2	E	150	ARG	CB-CG-CD	-5.03	98.52	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	208	ALA	Peptide
2	A	209	GLY	Peptide
2	D	207	ALA	Peptide
1	J	14	LEU	Peptide

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	C	379	0	361	27	0
1	G	377	0	355	23	0
1	J	376	0	352	30	0
1	X	372	0	354	15	0
2	A	511	0	527	35	0
2	D	505	0	531	37	0
2	E	517	0	538	37	0
2	H	526	0	551	38	0
3	A	10	0	0	0	0
3	C	5	0	0	1	0
3	D	10	0	0	1	0
3	E	15	0	0	5	0
3	H	20	0	0	0	0
3	X	5	0	0	0	0
4	A	10	0	0	0	0
4	C	9	0	0	1	0
4	D	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	3	0	0	0	0
4	G	6	0	0	0	0
4	H	7	0	0	1	0
4	J	6	0	0	0	0
4	X	5	0	0	0	0
All	All	3680	0	3569	197	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 27.

All (197) 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:H:205:ILE:HD13	2:H:205:ILE:O	1.37	1.25
1:J:12:PRO:N	1:J:13:PRO:CD	1.99	1.24
1:J:14:LEU:HD23	1:J:14:LEU:C	1.54	1.24
1:J:12:PRO:N	1:J:13:PRO:HD3	1.51	1.15
2:A:141:MSE:N	2:A:141:MSE:SE	2.30	1.15
1:C:13:PRO:HG2	3:C:101:SO4:O3	1.48	1.11
2:E:209:GLY:O	2:E:210:ASP:HB3	1.51	1.10
1:G:46:LEU:HG	2:E:151:MSE:CE	1.86	1.04
2:H:205:ILE:HD13	2:H:205:ILE:C	1.79	1.01
1:X:46:LEU:HG	2:D:151:MSE:CE	1.92	0.99
1:J:13:PRO:O	1:J:14:LEU:HB3	1.59	0.99
1:G:11:ARG:N	1:G:12:PRO:HD2	1.78	0.98
1:J:46:LEU:HG	2:H:151:MSE:CE	1.96	0.95
1:J:14:LEU:C	1:J:14:LEU:CD2	2.30	0.93
1:J:14:LEU:HD23	1:J:15:ASP:N	1.83	0.92
2:H:205:ILE:C	2:H:205:ILE:CD1	2.39	0.90
2:A:203:ASP:O	2:A:206:VAL:HG12	1.73	0.88
1:J:12:PRO:N	1:J:13:PRO:HD2	1.87	0.86
1:J:14:LEU:HD23	1:J:14:LEU:O	1.76	0.86
1:C:46:LEU:HG	2:A:151:MSE:CE	2.06	0.85
1:G:13:PRO:O	1:G:16:GLU:HB2	1.78	0.84
2:E:153:GLU:O	2:E:156:GLU:HG2	1.79	0.83
2:A:153:GLU:O	2:A:156:GLU:HG2	1.78	0.83
1:G:11:ARG:N	1:G:12:PRO:CD	2.44	0.81
2:E:157:ILE:HD13	2:E:204:GLU:CD	2.00	0.81
2:D:153:GLU:O	2:D:156:GLU:HG2	1.81	0.80
2:H:153:GLU:O	2:H:156:GLU:HG2	1.81	0.80
1:X:46:LEU:HG	2:D:151:MSE:HE1	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:O	1:C:14:LEU:CD2	2.31	0.77
1:C:12:PRO:CB	1:C:13:PRO:CD	2.63	0.77
1:G:46:LEU:HG	2:E:151:MSE:HE2	1.67	0.77
1:J:46:LEU:HG	2:H:151:MSE:HE1	1.66	0.77
1:G:46:LEU:HG	2:E:151:MSE:HE1	1.65	0.76
2:D:206:VAL:O	2:D:208:ALA:C	2.25	0.74
2:H:202:LYS:O	2:H:205:ILE:CG2	2.36	0.73
2:H:210:ASP:O	2:H:211:TYR:CB	2.37	0.73
2:H:203:ASP:O	2:H:206:VAL:HG12	1.89	0.71
2:E:209:GLY:O	2:E:210:ASP:CB	2.34	0.71
2:A:150:ARG:O	2:A:154:LEU:HD13	1.92	0.69
1:C:14:LEU:O	1:C:14:LEU:HD22	1.90	0.69
1:X:46:LEU:HG	2:D:151:MSE:HE2	1.75	0.69
1:J:14:LEU:CD2	1:J:14:LEU:O	2.37	0.69
1:J:13:PRO:O	1:J:14:LEU:CB	2.38	0.69
2:H:150:ARG:O	2:H:154:LEU:HD13	1.93	0.69
1:J:46:LEU:HD13	2:H:150:ARG:NH1	2.09	0.68
1:C:46:LEU:HD13	2:A:150:ARG:NH1	2.09	0.67
2:D:150:ARG:O	2:D:154:LEU:HD13	1.96	0.66
1:C:14:LEU:O	1:C:14:LEU:HD23	1.95	0.66
1:J:14:LEU:O	1:J:14:LEU:CG	2.45	0.65
2:H:202:LYS:O	2:H:205:ILE:HG22	1.97	0.65
1:X:13:PRO:O	1:X:16:GLU:HB2	1.96	0.65
1:G:46:LEU:CG	2:E:151:MSE:CE	2.71	0.65
2:D:157:ILE:HG21	2:D:204:GLU:OE2	1.97	0.64
2:E:150:ARG:O	2:E:154:LEU:HD13	1.97	0.64
2:E:207:ALA:O	2:E:208:ALA:HB3	1.98	0.63
2:E:185:SER:HB3	3:E:302:SO4:O3	2.00	0.62
2:D:207:ALA:HA	2:D:208:ALA:C	2.21	0.61
1:G:13:PRO:O	1:G:16:GLU:N	2.33	0.61
1:C:23:LEU:HD13	1:C:35:PHE:HZ	1.65	0.61
1:C:13:PRO:O	1:C:14:LEU:HB3	2.01	0.61
1:G:46:LEU:CG	2:E:151:MSE:HE1	2.31	0.61
1:X:23:LEU:HD22	1:X:23:LEU:O	2.01	0.60
1:C:46:LEU:HG	2:A:151:MSE:HE1	1.81	0.60
1:X:46:LEU:HD13	2:D:150:ARG:NH1	2.16	0.60
1:J:46:LEU:HG	2:H:151:MSE:HE2	1.80	0.60
1:J:14:LEU:O	1:J:14:LEU:HG	2.01	0.59
2:D:207:ALA:CA	2:D:208:ALA:C	2.71	0.59
1:C:12:PRO:HB3	1:C:13:PRO:CD	2.33	0.59
1:G:46:LEU:HD13	2:E:150:ARG:NH1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:154:LEU:HA	2:D:157:ILE:HD13	1.85	0.57
1:G:46:LEU:HD13	2:E:150:ARG:HH11	1.69	0.57
2:H:205:ILE:O	2:H:205:ILE:CD1	2.30	0.57
2:D:148:VAL:O	2:D:152:ASN:HB2	2.05	0.57
1:X:46:LEU:CG	2:D:151:MSE:HE1	2.35	0.56
1:G:23:LEU:HD22	1:G:23:LEU:O	2.06	0.56
1:C:13:PRO:O	1:C:14:LEU:CB	2.54	0.56
1:J:46:LEU:HD13	2:H:150:ARG:HH11	1.67	0.56
2:E:148:VAL:O	2:E:152:ASN:HB2	2.06	0.56
1:X:46:LEU:HD13	2:D:150:ARG:HH11	1.70	0.56
2:A:154:LEU:HA	2:A:157:ILE:HD13	1.88	0.55
2:D:157:ILE:HD12	2:D:157:ILE:H	1.71	0.55
1:J:12:PRO:CD	1:J:13:PRO:HD3	2.34	0.55
2:A:145:ALA:HB1	2:A:149:THR:HG22	1.88	0.55
2:E:185:SER:CB	3:E:302:SO4:O3	2.55	0.55
2:A:154:LEU:N	2:A:154:LEU:HD12	2.22	0.54
2:H:154:LEU:N	2:H:154:LEU:HD12	2.23	0.54
2:E:151:MSE:O	2:E:155:LEU:HG	2.07	0.54
1:J:46:LEU:CG	2:H:151:MSE:HE1	2.37	0.54
2:H:203:ASP:O	2:H:206:VAL:CG1	2.56	0.53
1:C:46:LEU:HD13	2:A:150:ARG:HH11	1.72	0.53
2:H:145:ALA:HB1	2:H:149:THR:HG22	1.89	0.53
1:C:12:PRO:HB3	1:C:13:PRO:HD3	1.90	0.53
2:D:185:SER:HB2	3:D:302:SO4:O4	2.09	0.53
2:D:196:ARG:NE	4:D:403:HOH:O	2.41	0.53
1:C:12:PRO:CB	1:C:13:PRO:HD3	2.39	0.53
2:A:157:ILE:HD12	2:A:157:ILE:H	1.72	0.52
1:J:57:PRO:O	1:J:58:PRO:C	2.46	0.52
2:H:202:LYS:O	2:H:205:ILE:HG23	2.07	0.52
2:A:156:GLU:HG2	2:A:157:ILE:HD12	1.91	0.52
1:C:20:THR:HG23	2:A:198:LEU:HD12	1.91	0.52
1:G:28:ALA:HB1	2:E:173:GLY:HA2	1.91	0.52
2:D:145:ALA:HB1	2:D:149:THR:CG2	2.40	0.52
1:G:46:LEU:CD2	2:E:151:MSE:HE1	2.40	0.52
2:H:145:ALA:HB1	2:H:149:THR:CG2	2.40	0.52
2:D:156:GLU:HG2	2:D:157:ILE:HD12	1.92	0.51
1:X:46:LEU:CG	2:D:151:MSE:CE	2.79	0.51
2:H:206:VAL:CG1	2:H:207:ALA:N	2.73	0.51
2:H:148:VAL:O	2:H:152:ASN:HB2	2.11	0.51
2:H:154:LEU:N	2:H:154:LEU:CD1	2.74	0.51
1:C:46:LEU:HG	2:A:151:MSE:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:148:VAL:O	2:A:152:ASN:HB2	2.11	0.50
2:E:154:LEU:N	2:E:154:LEU:HD12	2.25	0.50
2:A:203:ASP:O	2:A:206:VAL:CG1	2.55	0.50
2:A:154:LEU:N	2:A:154:LEU:CD1	2.75	0.50
2:A:145:ALA:HB1	2:A:149:THR:CG2	2.41	0.50
1:J:57:PRO:O	1:J:58:PRO:O	2.30	0.50
2:E:206:VAL:HG12	2:E:207:ALA:N	2.26	0.50
1:C:57:PRO:O	1:C:58:PRO:O	2.30	0.49
2:A:156:GLU:CG	2:A:157:ILE:HD12	2.42	0.49
2:D:151:MSE:O	2:D:155:LEU:HG	2.12	0.49
2:D:201:LEU:O	2:D:205:ILE:HG13	2.12	0.49
4:C:207:HOH:O	2:A:148:VAL:HG23	2.12	0.49
2:E:162:GLN:NE2	3:E:303:SO4:O4	2.45	0.49
2:A:150:ARG:O	2:A:153:GLU:HB3	2.13	0.48
2:E:154:LEU:N	2:E:154:LEU:CD1	2.76	0.48
2:E:145:ALA:HB1	2:E:149:THR:HG22	1.94	0.48
1:X:14:LEU:HA	1:X:14:LEU:HD22	1.67	0.47
2:D:204:GLU:O	2:D:207:ALA:O	2.33	0.47
1:J:50:TRP:CD2	2:H:151:MSE:HG2	2.49	0.47
2:E:145:ALA:HB1	2:E:149:THR:CG2	2.44	0.47
2:H:150:ARG:O	2:H:153:GLU:HB3	2.14	0.47
2:E:150:ARG:O	2:E:153:GLU:HB3	2.15	0.47
2:D:158:LEU:HD23	2:D:200:ARG:HG2	1.97	0.47
2:D:145:ALA:HB1	2:D:149:THR:HG22	1.96	0.47
1:C:14:LEU:CD2	1:C:14:LEU:C	2.83	0.47
2:D:150:ARG:O	2:D:153:GLU:HB3	2.15	0.46
1:G:46:LEU:CG	2:E:151:MSE:HE2	2.41	0.46
1:G:13:PRO:O	1:G:14:LEU:C	2.54	0.46
3:E:303:SO4:O2	1:J:13:PRO:O	2.33	0.46
1:J:20:THR:HG23	2:H:198:LEU:HD12	1.98	0.46
2:H:154:LEU:CD1	2:H:154:LEU:H	2.29	0.46
1:X:46:LEU:CD2	2:D:151:MSE:HE1	2.46	0.46
2:D:154:LEU:HD12	2:D:154:LEU:N	2.31	0.45
2:D:161:LYS:O	2:D:165:ILE:HG13	2.15	0.45
2:H:187:THR:O	2:H:191:ARG:HG3	2.17	0.45
2:A:201:LEU:O	2:A:205:ILE:HG13	2.17	0.45
1:C:12:PRO:HB2	1:C:13:PRO:CD	2.45	0.44
2:E:207:ALA:O	2:E:208:ALA:CB	2.64	0.44
2:D:156:GLU:CG	2:D:157:ILE:HD12	2.47	0.44
2:D:154:LEU:N	2:D:154:LEU:CD1	2.81	0.44
2:D:206:VAL:C	2:D:208:ALA:C	2.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LEU:CD1	2:A:150:ARG:HH11	2.31	0.44
1:C:46:LEU:CG	2:A:151:MSE:HE1	2.47	0.43
2:H:158:LEU:HD23	2:H:200:ARG:HG2	1.99	0.43
2:D:157:ILE:HD12	2:D:157:ILE:N	2.33	0.43
1:X:14:LEU:HB3	2:A:159:PRO:HB3	1.99	0.43
3:E:302:SO4:O2	2:H:188:GLY:HA2	2.18	0.43
1:J:46:LEU:CD1	2:H:150:ARG:HH11	2.30	0.43
2:A:154:LEU:CD1	2:A:154:LEU:H	2.32	0.43
1:C:12:PRO:CB	1:C:13:PRO:HD2	2.48	0.42
1:C:37:ASP:OD1	1:C:38:PRO:HD2	2.19	0.42
2:A:157:ILE:HD12	2:A:157:ILE:N	2.33	0.42
2:E:154:LEU:CD1	2:E:154:LEU:H	2.32	0.42
1:J:37:ASP:HA	1:J:38:PRO:HD3	1.85	0.42
1:C:50:TRP:CD2	2:A:151:MSE:HG2	2.54	0.42
2:E:156:GLU:HA	2:E:163:ARG:HH21	1.84	0.42
2:D:156:GLU:HA	2:D:163:ARG:HH21	1.84	0.42
1:C:46:LEU:CD2	2:A:151:MSE:HE1	2.50	0.42
1:X:55:ARG:O	1:X:57:PRO:HD3	2.20	0.42
2:A:158:LEU:HD23	2:A:200:ARG:HG2	2.01	0.42
1:G:20:THR:HG23	2:E:198:LEU:HD12	2.01	0.42
1:G:43:LEU:HD13	2:E:205:ILE:HD11	2.01	0.42
2:H:199:GLN:HB3	4:H:405:HOH:O	2.19	0.42
2:A:206:VAL:CG1	2:A:207:ALA:N	2.82	0.41
2:E:187:THR:CG2	2:E:191:ARG:HH11	2.32	0.41
1:X:43:LEU:HD13	2:D:205:ILE:HD11	2.01	0.41
2:D:156:GLU:HG3	2:D:157:ILE:N	2.36	0.41
2:A:201:LEU:O	2:A:205:ILE:CG1	2.69	0.41
1:G:14:LEU:HD12	1:G:14:LEU:HA	1.71	0.41
1:G:23:LEU:HD22	1:G:23:LEU:C	2.41	0.41
2:E:158:LEU:HD12	2:E:158:LEU:HA	1.92	0.41
2:H:150:ARG:HH11	2:H:150:ARG:HD3	1.60	0.41
2:H:203:ASP:O	2:H:206:VAL:CB	2.68	0.41
2:A:150:ARG:HH11	2:A:150:ARG:HD3	1.60	0.41
2:E:197:ALA:O	2:E:201:LEU:HB2	2.21	0.41
1:C:46:LEU:CG	2:A:151:MSE:CE	2.90	0.41
1:G:37:ASP:HA	1:G:38:PRO:HD3	1.83	0.41
1:J:46:LEU:CD2	2:H:151:MSE:HE1	2.51	0.41
1:X:23:LEU:HD22	1:X:23:LEU:C	2.41	0.40
2:D:187:THR:CG2	2:D:191:ARG:HH11	2.35	0.40
1:J:17:LEU:HD12	1:J:17:LEU:HA	1.89	0.40
2:E:156:GLU:HG3	2:E:157:ILE:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:187:THR:CG2	2:H:191:ARG:HH11	2.34	0.40
1:G:46:LEU:CD2	2:E:151:MSE:CE	2.99	0.40
1:G:56:TRP:HA	1:G:57:PRO:HD3	1.47	0.40
1:J:37:ASP:O	1:J:40:ASP:HB2	2.20	0.40
1:J:46:LEU:CG	2:H:151:MSE:CE	2.83	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	C	45/80 (56%)	43 (96%)	1 (2%)	1 (2%)	5 9
1	G	45/80 (56%)	44 (98%)	1 (2%)	0	100 100
1	J	45/80 (56%)	42 (93%)	2 (4%)	1 (2%)	5 9
1	X	44/80 (55%)	42 (96%)	2 (4%)	0	100 100
2	A	68/86 (79%)	67 (98%)	1 (2%)	0	100 100
2	D	66/86 (77%)	65 (98%)	1 (2%)	0	100 100
2	E	68/86 (79%)	67 (98%)	1 (2%)	0	100 100
2	H	69/86 (80%)	68 (99%)	1 (1%)	0	100 100
All	All	450/664 (68%)	438 (97%)	10 (2%)	2 (0%)	30 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	13	PRO
1	J	57	PRO

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	C	39/61 (64%)	35 (90%)	4 (10%)	6 12
1	G	38/61 (62%)	32 (84%)	6 (16%)	2 4
1	J	38/61 (62%)	34 (90%)	4 (10%)	5 11
1	X	38/61 (62%)	32 (84%)	6 (16%)	2 4
2	A	52/65 (80%)	45 (86%)	7 (14%)	3 6
2	D	52/65 (80%)	45 (86%)	7 (14%)	3 6
2	E	53/65 (82%)	46 (87%)	7 (13%)	3 6
2	H	54/65 (83%)	44 (82%)	10 (18%)	1 2
All	All	364/504 (72%)	313 (86%)	51 (14%)	3 5

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	14	LEU
1	X	16	GLU
1	X	17	LEU
1	X	20	THR
1	X	23	LEU
1	X	34	ASP
2	D	147	SER
2	D	149	THR
2	D	174	LEU
2	D	183	VAL
2	D	198	LEU
2	D	200	ARG
2	D	201	LEU
1	C	14	LEU
1	C	15	ASP
1	C	20	THR
1	C	34	ASP
2	A	141	MSE
2	A	149	THR

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Mol	Chain	Res	Type
2	A	174	LEU
2	A	198	LEU
2	A	200	ARG
2	A	201	LEU
2	A	205	ILE
1	G	14	LEU
1	G	16	GLU
1	G	17	LEU
1	G	20	THR
1	G	23	LEU
1	G	27	LEU
2	E	149	THR
2	E	158	LEU
2	E	174	LEU
2	E	198	LEU
2	E	200	ARG
2	E	201	LEU
2	E	210	ASP
1	J	14	LEU
1	J	17	LEU
1	J	20	THR
1	J	34	ASP
2	H	147	SER
2	H	149	THR
2	H	161	LYS
2	H	174	LEU
2	H	198	LEU
2	H	200	ARG
2	H	201	LEU
2	H	205	ILE
2	H	206	VAL
2	H	210	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	49	GLN
1	C	49	GLN
1	G	49	GLN
1	J	49	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 oligosaccharides in this entry.

5.6 Ligand geometry

13 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	SO4	H	303	-	4,4,4	0.20	0	6,6,6	0.38	0
3	SO4	E	302	-	4,4,4	0.38	0	6,6,6	0.35	0
3	SO4	D	302	-	4,4,4	0.35	0	6,6,6	0.28	0
3	SO4	D	301	-	4,4,4	0.24	0	6,6,6	0.44	0
3	SO4	H	304	-	4,4,4	0.26	0	6,6,6	0.20	0
3	SO4	X	101	-	4,4,4	0.27	0	6,6,6	0.14	0
3	SO4	E	303	-	4,4,4	0.39	0	6,6,6	0.55	0
3	SO4	E	301	-	4,4,4	0.28	0	6,6,6	0.29	0
3	SO4	C	101	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	A	302	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	A	301	-	4,4,4	0.27	0	6,6,6	0.44	0
3	SO4	H	301	-	4,4,4	0.28	0	6,6,6	0.19	0
3	SO4	H	302	-	4,4,4	0.37	0	6,6,6	0.31	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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	SO4	3	0
3	D	302	SO4	1	0
3	E	303	SO4	2	0
3	C	101	SO4	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	C	47/80 (58%)	-1.06	0 100 100	20, 49, 76, 89	0
1	G	47/80 (58%)	-0.91	0 100 100	34, 50, 78, 88	0
1	J	47/80 (58%)	-1.07	0 100 100	20, 49, 75, 87	0
1	X	46/80 (57%)	-0.94	0 100 100	34, 48, 76, 88	0
2	A	68/86 (79%)	-0.96	0 100 100	20, 51, 77, 82	0
2	D	66/86 (76%)	-1.02	0 100 100	28, 51, 73, 83	0
2	E	68/86 (79%)	-0.82	1 (1%) 71 68	31, 51, 77, 82	0
2	H	69/86 (80%)	-1.05	0 100 100	33, 53, 77, 83	0
All	All	458/664 (68%)	-0.98	1 (0%) 92 90	20, 51, 77, 89	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	171	VAL	3.6

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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	SO4	E	301	5/5	0.96	0.07	60,66,76,86	0
3	SO4	H	302	5/5	0.96	0.07	72,81,108,108	0
3	SO4	D	302	5/5	0.97	0.06	65,74,85,90	0
3	SO4	E	303	5/5	0.97	0.06	62,70,86,86	0
3	SO4	H	301	5/5	0.97	0.05	62,68,79,87	0
3	SO4	A	302	5/5	0.97	0.05	68,72,76,89	0
3	SO4	C	101	5/5	0.98	0.07	30,30,30,30	0
3	SO4	X	101	5/5	0.98	0.05	67,80,88,92	0
3	SO4	H	303	5/5	0.98	0.07	63,65,77,87	0
3	SO4	H	304	5/5	0.98	0.05	66,72,87,89	0
3	SO4	E	302	5/5	0.99	0.05	58,60,69,86	0
3	SO4	D	301	5/5	0.99	0.05	50,52,83,84	0
3	SO4	A	301	5/5	0.99	0.06	53,61,71,77	0

6.5 Other polymers (i)

There are no such residues in this entry.