Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:26 AM BST

PDB ID	:	6SN1
Title	:	Crystal structure of the human INTS13-INTS14 complex
Authors	:	Jonas, S.; Sabath, K.; Staeubli, M.L.
Deposited on	:	2019-08-23
Resolution	:	2.54 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 following versions of software and data (see references ⓘ) were used in the production of this report:

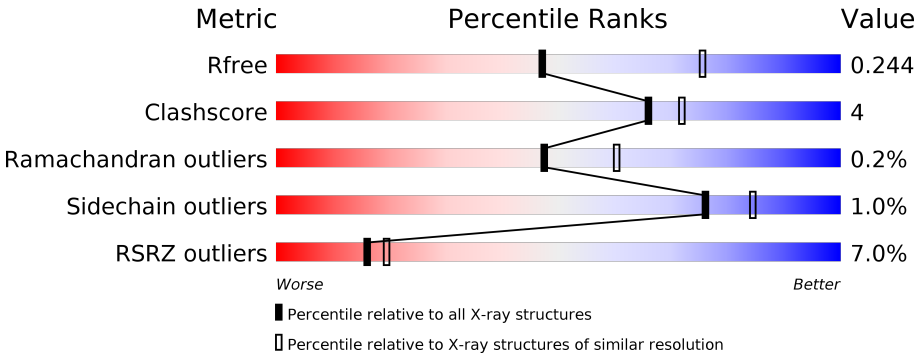
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 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	763	5% 59% 8% 32%
2	B	518	7% 86% 10% .

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	B	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8015 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 Integrator complex subunit 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4039	2535	705	767	32			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-56	MET	-	initiating methionine	UNP Q9NVM9
A	-55	ALA	-	expression tag	UNP Q9NVM9
A	-54	SER	-	expression tag	UNP Q9NVM9
A	-53	ALA	-	expression tag	UNP Q9NVM9
A	-52	TRP	-	expression tag	UNP Q9NVM9
A	-51	SER	-	expression tag	UNP Q9NVM9
A	-50	HIS	-	expression tag	UNP Q9NVM9
A	-49	PRO	-	expression tag	UNP Q9NVM9
A	-48	GLN	-	expression tag	UNP Q9NVM9
A	-47	PHE	-	expression tag	UNP Q9NVM9
A	-46	GLU	-	expression tag	UNP Q9NVM9
A	-45	LYS	-	expression tag	UNP Q9NVM9
A	-44	GLY	-	expression tag	UNP Q9NVM9
A	-43	GLY	-	expression tag	UNP Q9NVM9
A	-42	GLY	-	expression tag	UNP Q9NVM9
A	-41	SER	-	expression tag	UNP Q9NVM9
A	-40	GLY	-	expression tag	UNP Q9NVM9
A	-39	GLY	-	expression tag	UNP Q9NVM9
A	-38	GLY	-	expression tag	UNP Q9NVM9
A	-37	SER	-	expression tag	UNP Q9NVM9
A	-36	GLY	-	expression tag	UNP Q9NVM9
A	-35	GLY	-	expression tag	UNP Q9NVM9
A	-34	SER	-	expression tag	UNP Q9NVM9
A	-33	ALA	-	expression tag	UNP Q9NVM9
A	-32	TRP	-	expression tag	UNP Q9NVM9
A	-31	SER	-	expression tag	UNP Q9NVM9
A	-30	HIS	-	expression tag	UNP Q9NVM9

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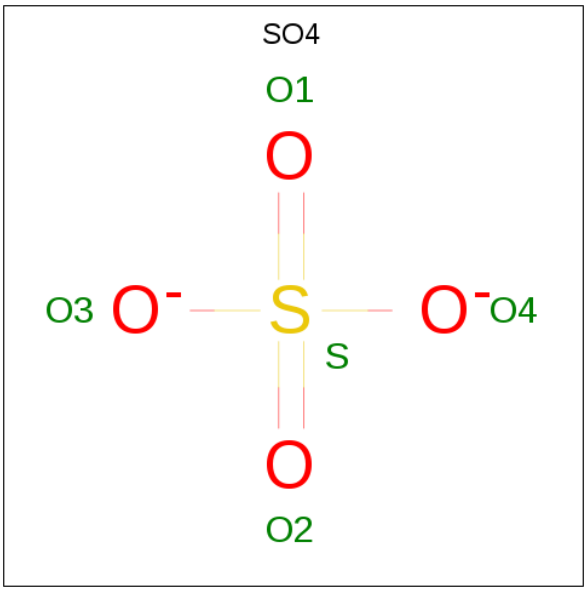
Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	PRO	-	expression tag	UNP Q9NVM9
A	-28	GLN	-	expression tag	UNP Q9NVM9
A	-27	PHE	-	expression tag	UNP Q9NVM9
A	-26	GLU	-	expression tag	UNP Q9NVM9
A	-25	LYS	-	expression tag	UNP Q9NVM9
A	-24	SER	-	expression tag	UNP Q9NVM9
A	-23	SER	-	expression tag	UNP Q9NVM9
A	-22	GLY	-	expression tag	UNP Q9NVM9
A	-21	SER	-	expression tag	UNP Q9NVM9
A	-20	GLY	-	expression tag	UNP Q9NVM9
A	-19	SER	-	expression tag	UNP Q9NVM9
A	-18	GLY	-	expression tag	UNP Q9NVM9
A	-17	LEU	-	expression tag	UNP Q9NVM9
A	-16	GLU	-	expression tag	UNP Q9NVM9
A	-15	VAL	-	expression tag	UNP Q9NVM9
A	-14	LEU	-	expression tag	UNP Q9NVM9
A	-13	PHE	-	expression tag	UNP Q9NVM9
A	-12	GLN	-	expression tag	UNP Q9NVM9
A	-11	GLY	-	expression tag	UNP Q9NVM9
A	-10	PRO	-	expression tag	UNP Q9NVM9
A	-9	SER	-	expression tag	UNP Q9NVM9
A	-8	ASP	-	expression tag	UNP Q9NVM9
A	-7	PRO	-	expression tag	UNP Q9NVM9
A	-6	GLY	-	expression tag	UNP Q9NVM9
A	-5	PRO	-	expression tag	UNP Q9NVM9
A	-4	LYS	-	expression tag	UNP Q9NVM9
A	-3	ARG	-	expression tag	UNP Q9NVM9
A	-2	ALA	-	expression tag	UNP Q9NVM9
A	-1	GLU	-	expression tag	UNP Q9NVM9
A	0	PHE	-	expression tag	UNP Q9NVM9

- Molecule 2 is a protein called Integrator complex subunit 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	503	3856	2466	637	728	25	0	0	0

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



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

- Molecule 4 is water.

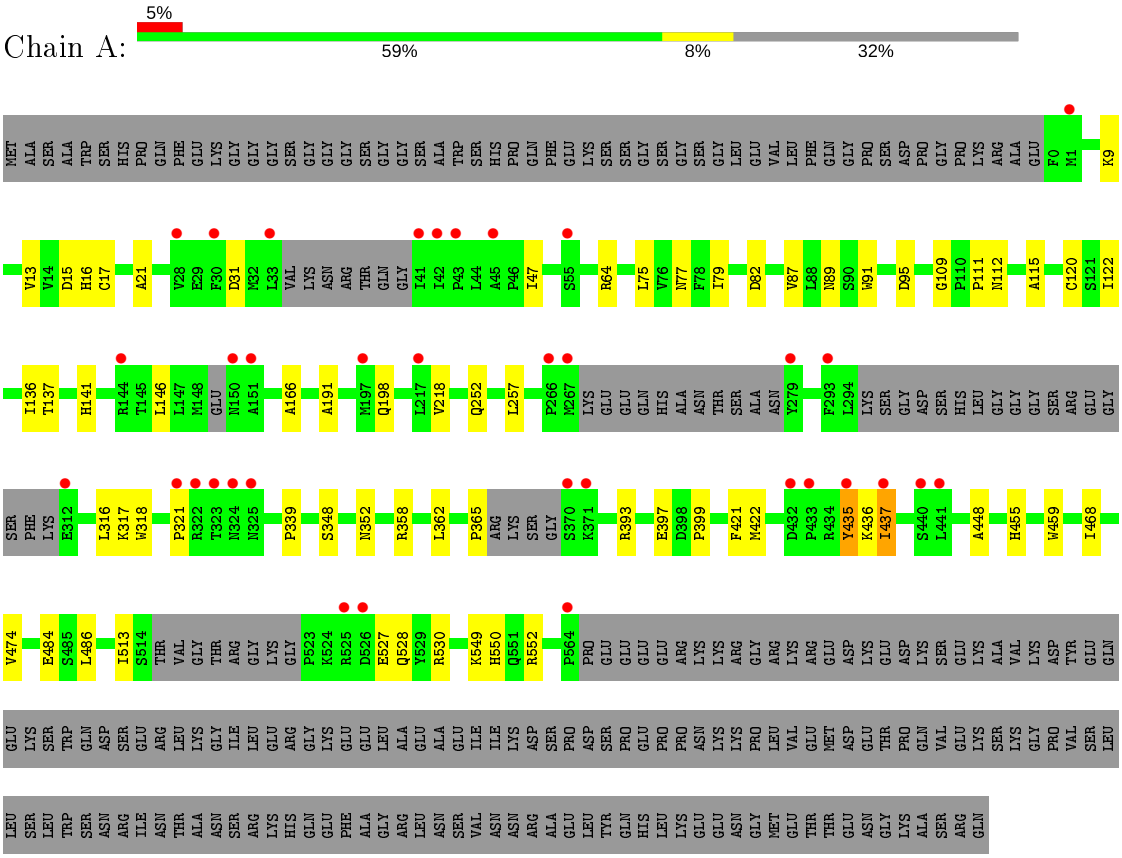
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O 37 37	0	0
4	B	53	Total O 53 53	0	0

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.

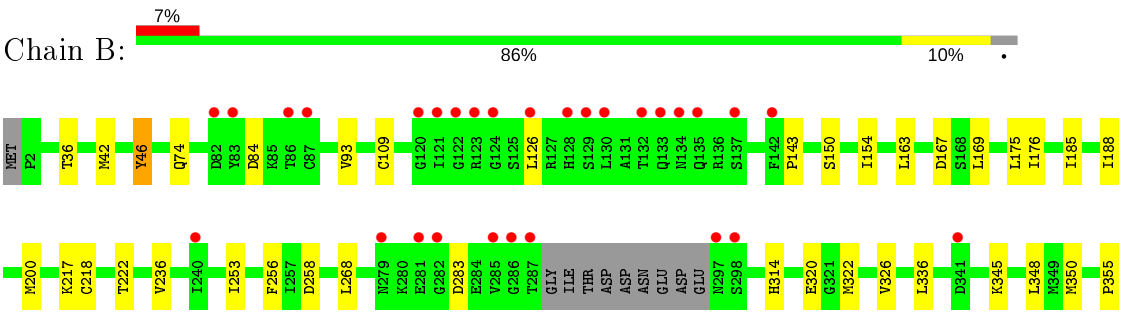
- Molecule 1: Integrator complex subunit 13

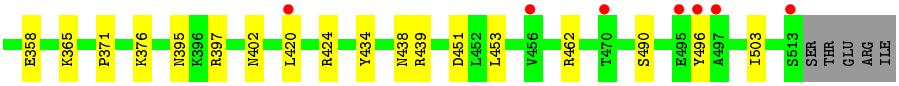
Chain A:



- Molecule 2: Integrator complex subunit 14

Chain B:




E358
K365
P371
K376
N395
K396
R397
N402
L420
R424
Y434
N438
R439
D451
L452
L453
V456
R462
T470
S490
E495
Y496
A497
I503
S513
SER
THR
GLU
ARG
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	190.99Å 115.35Å 147.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.47 – 2.54 45.47 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.47-2.54) 88.5 (45.47-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.51 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.224 , 0.244 0.224 , 0.244	Depositor DCC
R_{free} test set	5463 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8015	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	A	0.23	0/4118	0.40	0/5588
2	B	0.25	0/3943	0.42	0/5365
All	All	0.24	0/8061	0.41	0/10953

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	4039	0	3931	35	0
2	B	3856	0	3813	33	0
3	A	20	0	0	0	0
3	B	10	0	0	3	0
4	A	37	0	0	0	0
4	B	53	0	0	0	0
All	All	8015	0	7744	63	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 4.

All (63) 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:A:513:ILE:HD13	1:A:528:GLN:HG2	1.74	0.69
1:A:348:SER:O	1:A:352:ASN:ND2	2.33	0.62
1:A:317:LYS:HE3	1:A:365:PRO:HB3	1.80	0.62
2:B:217:LYS:HG2	2:B:222:THR:HG22	1.81	0.62
1:A:435:TYR:HD1	1:A:436:LYS:H	1.47	0.62
1:A:64:ARG:NH1	1:A:339:PRO:O	2.33	0.61
1:A:9:LYS:HE2	1:A:137:THR:HG23	1.81	0.60
1:A:435:TYR:HD1	1:A:437:ILE:H	1.49	0.60
1:A:47:ILE:HG12	2:B:451:ASP:HB3	1.84	0.59
1:A:15:ASP:HB3	1:A:122:ILE:HD13	1.85	0.57
1:A:112:ASN:HB3	1:A:115:ALA:HB2	1.88	0.56
2:B:439:ARG:NH2	3:B:602:SO4:O2	2.37	0.56
2:B:176:ILE:HD12	2:B:185:ILE:HG12	1.89	0.54
2:B:163:LEU:HB3	2:B:169:LEU:HB2	1.89	0.54
2:B:126:LEU:HD11	2:B:175:LEU:HD21	1.90	0.53
2:B:268:LEU:HD11	2:B:355:PRO:HD3	1.91	0.52
1:A:79:ILE:HG12	1:A:87:VAL:HG12	1.92	0.51
2:B:154:ILE:HB	2:B:185:ILE:HD13	1.93	0.51
2:B:283:ASP:N	2:B:283:ASP:OD1	2.41	0.51
1:A:527:GLU:OE1	1:A:530:ARG:NH2	2.44	0.50
1:A:252:GLN:HA	1:A:257:LEU:HB2	1.93	0.50
2:B:320:GLU:HB3	2:B:322:MET:HE3	1.94	0.49
1:A:316:LEU:HB3	1:A:362:LEU:HB3	1.96	0.48
1:A:421:PHE:HE1	1:A:455:HIS:HB3	1.77	0.48
1:A:136:ILE:HD13	1:A:141:HIS:HB2	1.95	0.48
2:B:109:CYS:O	2:B:150:SER:HA	2.15	0.47
2:B:42:MET:HG3	2:B:46:TYR:HB3	1.96	0.46
2:B:453:LEU:HB2	2:B:490:SER:HB3	1.98	0.46
1:A:191:ALA:HB2	1:A:198:GLN:NE2	2.31	0.46
1:A:549:LYS:HG2	1:A:552:ARG:NH2	2.31	0.46
2:B:376:LYS:HB2	2:B:376:LYS:HE2	1.80	0.45
2:B:93:VAL:HG23	2:B:143:PRO:HG3	1.99	0.45
2:B:314:HIS:HB2	2:B:348:LEU:HB2	1.99	0.45
1:A:21:ALA:HB2	1:A:111:PRO:HG2	1.98	0.45
1:A:31:ASP:OD2	2:B:462:ARG:NH2	2.49	0.45
2:B:395:ASN:N	3:B:601:SO4:O1	2.33	0.45
1:A:17:CYS:SG	1:A:120:CYS:HB3	2.57	0.44
1:A:13:VAL:HG12	1:A:122:ILE:HD11	2.00	0.44
1:A:166:ALA:HB3	1:A:218:VAL:HG21	1.99	0.44
2:B:336:LEU:HD23	2:B:350:MET:HB2	2.00	0.44
2:B:258:ASP:HA	2:B:322:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:HB2	1:A:358:ARG:HH21	1.82	0.43
1:A:89:ASN:HB2	1:A:95:ASP:HB3	2.00	0.42
2:B:36:THR:HA	2:B:74:GLN:HE22	1.85	0.42
1:A:468:ILE:HB	1:A:474:VAL:HG11	2.01	0.42
2:B:218:CYS:HB2	2:B:253:ILE:HD12	2.02	0.42
1:A:448:ALA:HA	2:B:371:PRO:HG3	2.01	0.42
2:B:496:TYR:CD2	2:B:503:ILE:HG12	2.55	0.42
1:A:399:PRO:HD2	2:B:345:LYS:HB3	2.02	0.42
2:B:397:ARG:NH2	3:B:601:SO4:O3	2.41	0.42
2:B:188:ILE:HG13	2:B:200:MET:HE3	2.02	0.42
1:A:16:HIS:NE2	1:A:109:GLY:O	2.50	0.41
1:A:393:ARG:NH2	1:A:397:GLU:OE1	2.50	0.41
2:B:434:TYR:O	2:B:438:ASN:ND2	2.43	0.41
2:B:402:ASN:OD1	2:B:439:ARG:HD3	2.21	0.41
1:A:318:TRP:HE1	1:A:321:PRO:HD3	1.86	0.41
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.89	0.40
1:A:422:MET:HG2	2:B:256:PHE:CE2	2.57	0.40
1:A:486:LEU:HG	1:A:550:HIS:CE1	2.56	0.40
2:B:420:LEU:HD23	2:B:424:ARG:HH22	1.85	0.40
1:A:75:LEU:HD13	1:A:91:TRP:O	2.21	0.40
2:B:358:GLU:HG3	2:B:365:LYS:HG2	2.03	0.40
2:B:402:ASN:ND2	2:B:439:ARG:HH21	2.19	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	503/763 (66%)	489 (97%)	13 (3%)	1 (0%)	47	60
2	B	499/518 (96%)	478 (96%)	20 (4%)	1 (0%)	47	60
All	All	1002/1281 (78%)	967 (96%)	33 (3%)	2 (0%)	47	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	ILE
2	B	236	VAL

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	453/679 (67%)	448 (99%)	5 (1%)	73 83
2	B	423/452 (94%)	419 (99%)	4 (1%)	78 86
All	All	876/1131 (78%)	867 (99%)	9 (1%)	76 84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	82	ASP
1	A	435	TYR
1	A	459	TRP
1	A	484	GLU
2	B	46	TYR
2	B	84	ASP
2	B	167	ASP
2	B	326	VAL

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

Mol	Chain	Res	Type
1	A	77	ASN
1	A	528	GLN
2	B	74	GLN
2	B	402	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 monosaccharides in this entry.

5.6 Ligand geometry

6 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	A	801	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	802	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	804	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	601	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.05	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	SO4	2	0
3	B	602	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	A	517/763 (67%)	0.33	35 (6%)	17	20	48, 77, 140, 174	0
2	B	503/518 (97%)	0.36	36 (7%)	15	18	46, 72, 144, 190	0
All	All	1020/1281 (79%)	0.34	71 (6%)	16	19	46, 75, 143, 190	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	137	SER	7.0
1	A	370	SER	5.7
2	B	287	THR	5.4
2	B	135	GLN	4.8
1	A	437	ILE	4.8
2	B	121	ILE	4.6
2	B	496	TYR	4.4
1	A	42	ILE	4.4
2	B	240	ILE	4.3
1	A	441	LEU	4.0
1	A	1	MET	3.8
1	A	41	ILE	3.8
2	B	286	GLY	3.8
1	A	433	PRO	3.7
1	A	440	SER	3.7
2	B	142	PHE	3.7
2	B	120	GLY	3.6
2	B	124	GLY	3.6
1	A	325	ASN	3.6
1	A	432	ASP	3.6
1	A	312	GLU	3.4
2	B	297	ASN	3.3
1	A	279	TYR	3.3
2	B	133	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	217	LEU	3.2
2	B	298	SER	3.2
2	B	126	LEU	3.1
2	B	134	ASN	3.0
1	A	321	PRO	3.0
2	B	470	THR	2.9
1	A	526	ASP	2.9
1	A	45	ALA	2.9
2	B	285	VAL	2.8
1	A	151	ALA	2.8
1	A	43	PRO	2.8
2	B	497	ALA	2.8
2	B	132	THR	2.8
2	B	130	LEU	2.8
2	B	83	TYR	2.7
1	A	323	THR	2.7
1	A	435	TYR	2.6
2	B	513	SER	2.6
1	A	266	PRO	2.6
1	A	371	LYS	2.6
1	A	564	PRO	2.6
1	A	324	ASN	2.6
2	B	456	VAL	2.6
1	A	150	ASN	2.5
2	B	128	HIS	2.5
2	B	281	GLU	2.5
1	A	267	MET	2.4
1	A	322	ARG	2.3
2	B	123	ARG	2.3
2	B	282	GLY	2.2
1	A	197	MET	2.2
1	A	525	ARG	2.2
1	A	144	ARG	2.2
2	B	122	GLY	2.1
2	B	495	GLU	2.1
1	A	28	VAL	2.1
1	A	293	PHE	2.1
1	A	33	LEU	2.1
2	B	87	CYS	2.1
2	B	420	LEU	2.1
2	B	279	ASN	2.1
2	B	82	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	86	THR	2.0
1	A	30	PHE	2.0
2	B	129	SER	2.0
1	A	55	SER	2.0
2	B	341	ASP	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	SO4	A	803	5/5	0.74	0.25	153,155,163,174	0
3	SO4	A	801	5/5	0.77	0.18	209,210,213,219	0
3	SO4	B	602	5/5	0.79	0.21	242,244,246,258	0
3	SO4	A	804	5/5	0.85	0.34	169,170,173,207	0
3	SO4	A	802	5/5	0.89	0.32	198,203,217,221	0
3	SO4	B	601	5/5	0.90	0.19	123,124,151,160	0

6.5 Other polymers (i)

There are no such residues in this entry.