



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2016 – 12:04 AM EST

PDB ID : 2PVY
Title : Crystal Structure of FGF Receptor 2 (FGFR2) Kinase Domain Harboring the Pathogenic K659N Mutation Responsible for an Unclassified Craniosynostosis Syndrome.
Authors : Chen, H.; Mohammadi, M.
Deposited on : 2007-05-10
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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

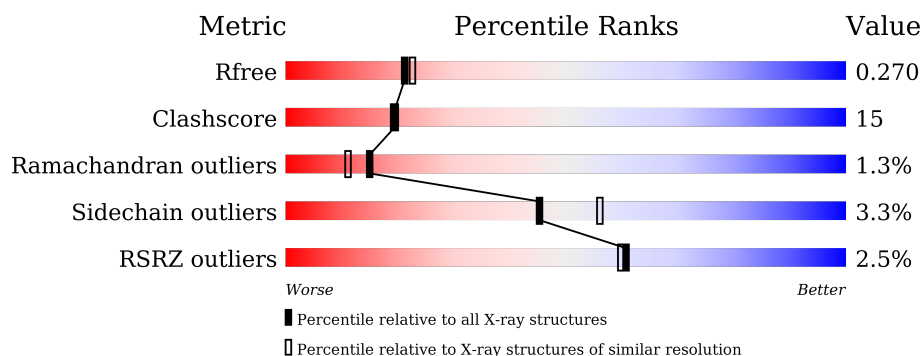
1 Overall quality at a glance

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 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 $\leq 5\%$. 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	324	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>22%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	324	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>23%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	324	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	324	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>23%</div> <div>••</div> <div>13%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACP	A	802	-	-	-	X
3	ACP	B	8002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9429 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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2280	1449	390	421	20			
1	B	286	Total	C	N	O	S	0	0	0
			2278	1452	389	417	20			
1	C	285	Total	C	N	O	S	0	0	0
			2270	1448	385	416	21			
1	D	283	Total	C	N	O	S	0	0	0
			2246	1431	382	413	20			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	EXPRESSION TAG	UNP P21802
A	446	GLY	-	EXPRESSION TAG	UNP P21802
A	447	SER	-	EXPRESSION TAG	UNP P21802
A	448	SER	-	EXPRESSION TAG	UNP P21802
A	449	HIS	-	EXPRESSION TAG	UNP P21802
A	450	HIS	-	EXPRESSION TAG	UNP P21802
A	451	HIS	-	EXPRESSION TAG	UNP P21802
A	452	HIS	-	EXPRESSION TAG	UNP P21802
A	453	HIS	-	EXPRESSION TAG	UNP P21802
A	454	HIS	-	EXPRESSION TAG	UNP P21802
A	455	SER	-	EXPRESSION TAG	UNP P21802
A	456	GLN	-	EXPRESSION TAG	UNP P21802
A	457	ASP	-	EXPRESSION TAG	UNP P21802
A	491	ALA	CYS	ENGINEERED	UNP P21802
A	659	ASN	LYS	ENGINEERED	UNP P21802
B	445	MET	-	EXPRESSION TAG	UNP P21802
B	446	GLY	-	EXPRESSION TAG	UNP P21802
B	447	SER	-	EXPRESSION TAG	UNP P21802
B	448	SER	-	EXPRESSION TAG	UNP P21802
B	449	HIS	-	EXPRESSION TAG	UNP P21802
B	450	HIS	-	EXPRESSION TAG	UNP P21802

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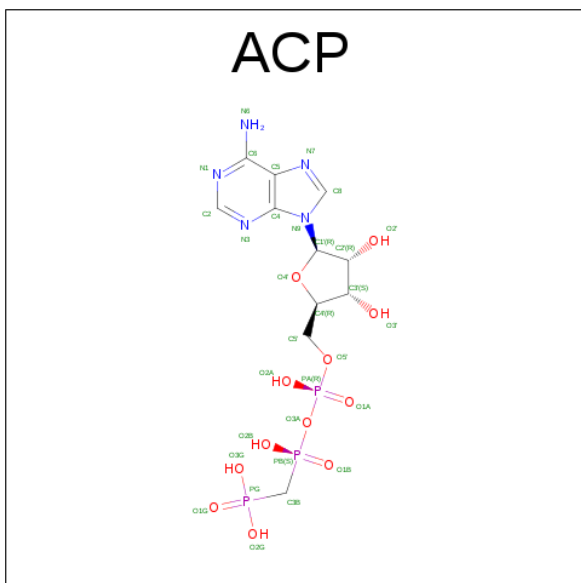
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	EXPRESSION TAG	UNP P21802
B	452	HIS	-	EXPRESSION TAG	UNP P21802
B	453	HIS	-	EXPRESSION TAG	UNP P21802
B	454	HIS	-	EXPRESSION TAG	UNP P21802
B	455	SER	-	EXPRESSION TAG	UNP P21802
B	456	GLN	-	EXPRESSION TAG	UNP P21802
B	457	ASP	-	EXPRESSION TAG	UNP P21802
B	491	ALA	CYS	ENGINEERED	UNP P21802
B	659	ASN	LYS	ENGINEERED	UNP P21802
C	445	MET	-	EXPRESSION TAG	UNP P21802
C	446	GLY	-	EXPRESSION TAG	UNP P21802
C	447	SER	-	EXPRESSION TAG	UNP P21802
C	448	SER	-	EXPRESSION TAG	UNP P21802
C	449	HIS	-	EXPRESSION TAG	UNP P21802
C	450	HIS	-	EXPRESSION TAG	UNP P21802
C	451	HIS	-	EXPRESSION TAG	UNP P21802
C	452	HIS	-	EXPRESSION TAG	UNP P21802
C	453	HIS	-	EXPRESSION TAG	UNP P21802
C	454	HIS	-	EXPRESSION TAG	UNP P21802
C	455	SER	-	EXPRESSION TAG	UNP P21802
C	456	GLN	-	EXPRESSION TAG	UNP P21802
C	457	ASP	-	EXPRESSION TAG	UNP P21802
C	491	ALA	CYS	ENGINEERED	UNP P21802
C	659	ASN	LYS	ENGINEERED	UNP P21802
D	445	MET	-	EXPRESSION TAG	UNP P21802
D	446	GLY	-	EXPRESSION TAG	UNP P21802
D	447	SER	-	EXPRESSION TAG	UNP P21802
D	448	SER	-	EXPRESSION TAG	UNP P21802
D	449	HIS	-	EXPRESSION TAG	UNP P21802
D	450	HIS	-	EXPRESSION TAG	UNP P21802
D	451	HIS	-	EXPRESSION TAG	UNP P21802
D	452	HIS	-	EXPRESSION TAG	UNP P21802
D	453	HIS	-	EXPRESSION TAG	UNP P21802
D	454	HIS	-	EXPRESSION TAG	UNP P21802
D	455	SER	-	EXPRESSION TAG	UNP P21802
D	456	GLN	-	EXPRESSION TAG	UNP P21802
D	457	ASP	-	EXPRESSION TAG	UNP P21802
D	491	ALA	CYS	ENGINEERED	UNP P21802
D	659	ASN	LYS	ENGINEERED	UNP P21802

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

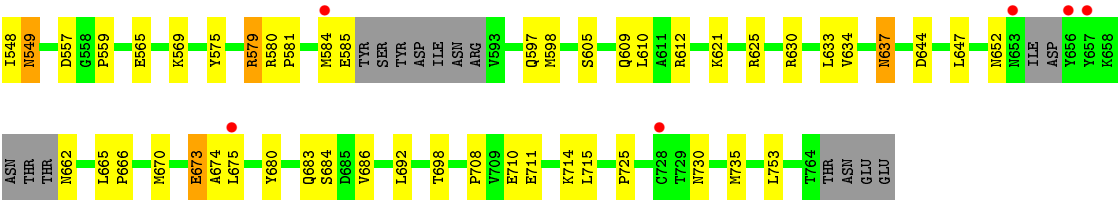
- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



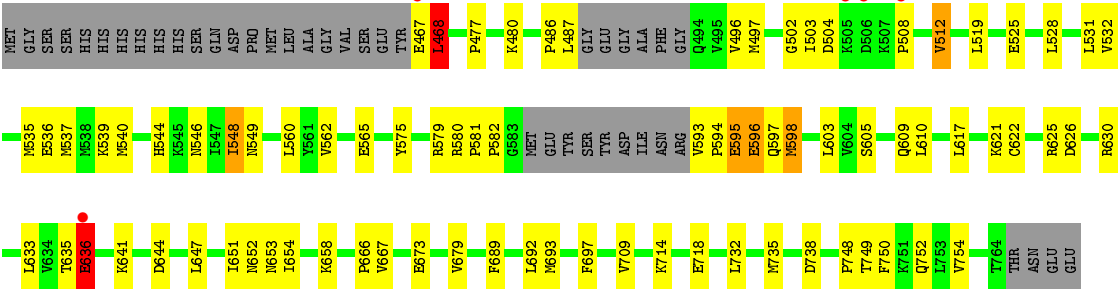
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O P 31 11 5 12 3	0	0
3	C	1	Total C N O 17 9 5 3	0	0
3	D	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	74	Total O 74 74	0	0
4	B	51	Total O 51 51	0	0
4	C	44	Total O 44 44	0	0
4	D	84	Total O 84 84	0	0



• Molecule 1: Fibroblast growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.58Å 70.47Å 85.69Å 92.19° 112.31° 116.19°	Depositor
Resolution (Å)	25.00 – 2.20 42.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.20) 87.8 (42.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.49 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.276 0.231 , 0.270	Depositor DCC
R_{free} test set	3283 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.058 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9429	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, 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	0.37	0/2327	0.64	0/3151
1	B	0.36	0/2324	0.60	0/3138
1	C	0.35	0/2316	0.58	0/3127
1	D	0.37	0/2293	0.62	0/3104
All	All	0.36	0/9260	0.61	0/12520

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 [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	2280	0	2257	70	0
1	B	2278	0	2275	75	0
1	C	2270	0	2269	71	0
1	D	2246	0	2239	73	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	17	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	14	0	0
3	C	17	0	9	0	0
3	D	17	0	9	0	0
4	A	74	0	0	3	0
4	B	51	0	0	1	0
4	C	44	0	0	0	0
4	D	84	0	0	1	0
All	All	9429	0	9081	273	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 15.

All (273) 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:735:MET:HE2	1:B:753:LEU:HD22	1.48	0.94
1:B:463:VAL:HG13	1:B:528:LEU:HD23	1.50	0.94
1:A:595:GLU:HG3	1:D:636:GLU:HB3	1.50	0.94
1:C:580:ARG:HD3	1:C:584:MET:HG2	1.51	0.90
1:A:549:ASN:H	1:A:549:ASN:HD22	0.95	0.89
1:A:661:THR:HA	1:A:678:ARG:HD3	1.54	0.88
1:D:667:VAL:HG21	1:D:709:VAL:HG13	1.54	0.87
1:B:540:MET:HE1	1:B:650:ASP:HB2	1.61	0.82
1:A:549:ASN:N	1:A:549:ASN:HD22	1.72	0.80
1:D:630:ARG:NH2	1:D:666:PRO:HG2	1.97	0.80
1:D:625:ARG:HD3	1:D:647:LEU:O	1.82	0.79
1:A:595:GLU:CG	1:D:636:GLU:HB3	2.12	0.78
1:B:617:LEU:HD11	1:B:622:CYS:SG	2.22	0.78
1:C:463:VAL:HG13	1:C:528:LEU:HD23	1.64	0.77
1:A:595:GLU:OE2	1:D:636:GLU:HA	1.85	0.76
1:B:665:LEU:HD12	1:B:670:MET:HE3	1.66	0.75
1:B:630:ARG:NH2	1:B:666:PRO:HG2	2.02	0.74
1:A:549:ASN:H	1:A:549:ASN:ND2	1.78	0.74
1:C:503:ILE:CG2	1:C:512:VAL:HG11	2.17	0.73
1:D:575:TYR:O	1:D:579:ARG:HG2	1.88	0.73
1:D:596:GLU:HG3	1:D:597:GLN:N	2.02	0.73
1:A:625:ARG:HD3	1:A:647:LEU:O	1.87	0.73
1:C:630:ARG:NH2	1:C:666:PRO:HG2	2.03	0.73
1:A:548:ILE:HG13	1:A:633:LEU:HD12	1.70	0.73
1:C:548:ILE:HG13	1:C:633:LEU:HD12	1.69	0.72
1:C:711:GLU:HB3	1:C:714:LYS:HE2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:THR:HG21	1:A:641:LYS:HE2	1.73	0.71
1:C:711:GLU:O	1:C:714:LYS:HG2	1.91	0.71
1:B:759:ARG:NH2	1:B:759:ARG:HB3	2.05	0.71
1:D:714:LYS:O	1:D:718:GLU:HG3	1.91	0.71
1:B:462:GLY:O	1:B:466:TYR:HB2	1.91	0.71
1:B:735:MET:CE	1:B:753:LEU:HD22	2.20	0.71
1:B:675:LEU:HD12	1:B:675:LEU:H	1.56	0.70
1:C:487:LEU:HD21	1:C:497:MET:HB2	1.73	0.70
1:C:503:ILE:HG21	1:C:512:VAL:HG11	1.74	0.69
1:B:519:LEU:HD11	1:B:528:LEU:HD13	1.74	0.69
1:A:661:THR:HG22	1:C:462:GLY:N	2.08	0.69
1:C:575:TYR:O	1:C:579:ARG:HD2	1.94	0.68
1:D:467:GLU:O	1:D:468:LEU:HB2	1.92	0.68
1:B:545:LYS:NZ	1:B:546:ASN:HD21	1.92	0.68
1:A:630:ARG:NH2	1:A:666:PRO:HG2	2.08	0.67
1:A:525:GLU:OE2	1:C:675:LEU:HD11	1.94	0.67
1:C:683:GLN:O	1:C:686:VAL:HG12	1.95	0.67
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.76	0.66
1:C:462:GLY:O	1:C:466:TYR:HB2	1.94	0.66
1:D:535:MET:CE	1:D:562:VAL:HG22	2.25	0.66
1:D:596:GLU:HG3	1:D:597:GLN:H	1.60	0.66
1:A:575:TYR:O	1:A:579:ARG:HD2	1.97	0.65
1:C:549:ASN:H	1:C:549:ASN:HD22	1.44	0.65
1:C:637:ASN:H	1:C:637:ASN:HD22	1.44	0.65
1:A:673:GLU:HB3	1:A:679:VAL:CG2	2.27	0.64
1:B:665:LEU:HD12	1:B:670:MET:CE	2.27	0.64
1:D:535:MET:HE3	1:D:562:VAL:HG22	1.78	0.64
1:B:503:ILE:HG22	1:B:512:VAL:HG11	1.79	0.64
1:C:683:GLN:HA	1:C:686:VAL:HG12	1.79	0.64
1:A:710:GLU:HG3	1:C:559:PRO:HA	1.79	0.64
1:B:540:MET:CE	1:B:650:ASP:HB2	2.28	0.64
1:A:537:MET:O	1:A:541:ILE:HG13	1.97	0.63
1:A:549:ASN:HB3	4:A:940:HOH:O	1.98	0.63
1:D:689:PHE:HE2	1:D:693:MET:HE2	1.63	0.63
1:B:575:TYR:O	1:B:579:ARG:CD	2.46	0.63
1:C:507:LYS:N	1:C:508:PRO:HD3	2.14	0.63
1:C:549:ASN:ND2	1:C:565:GLU:OE1	2.33	0.62
1:A:486:PRO:HA	1:A:496:VAL:HA	1.81	0.62
1:C:637:ASN:ND2	1:C:637:ASN:H	1.98	0.62
1:D:598:MET:HG2	1:D:603:LEU:CD2	2.30	0.62
1:C:630:ARG:HH21	1:C:666:PRO:HG2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:VAL:CG1	1:C:528:LEU:HD23	2.30	0.61
1:A:572:LEU:HD13	1:A:640:MET:HE3	1.81	0.61
1:A:606:CYS:SG	1:A:640:MET:HE2	2.41	0.61
1:C:708:PRO:HB2	1:C:710:GLU:OE1	2.00	0.61
1:B:575:TYR:O	1:B:579:ARG:HD3	2.00	0.60
1:B:545:LYS:HE2	1:B:639:VAL:HG13	1.83	0.60
1:C:581:PRO:HG3	1:C:597:GLN:NE2	2.17	0.60
1:D:651:ILE:HG22	1:D:654:ILE:HD11	1.84	0.60
1:B:463:VAL:CG1	1:B:528:LEU:HD23	2.29	0.59
1:D:503:ILE:HG22	1:D:512:VAL:HG11	1.83	0.59
1:D:579:ARG:CD	1:D:595:GLU:HB3	2.32	0.59
1:A:615:GLU:OE2	1:A:751:LYS:HA	2.02	0.59
1:B:507:LYS:N	1:B:508:PRO:HD3	2.17	0.58
1:D:579:ARG:HD3	1:D:595:GLU:HB3	1.85	0.58
1:A:502:GLY:C	1:A:504:ASP:H	2.06	0.58
1:B:535:MET:CE	1:B:560:LEU:HD11	2.33	0.58
1:A:506:ASP:O	1:A:508:PRO:HD3	2.04	0.58
1:A:606:CYS:SG	1:A:640:MET:CE	2.92	0.58
1:C:519:LEU:HD11	1:C:528:LEU:HD13	1.86	0.58
1:D:667:VAL:HG21	1:D:709:VAL:CG1	2.31	0.58
1:C:500:ALA:O	1:C:512:VAL:HG12	2.04	0.58
1:A:595:GLU:OE2	1:D:636:GLU:CA	2.52	0.58
1:B:569:LYS:HB2	1:B:634:VAL:O	2.04	0.57
1:B:675:LEU:HD12	1:B:675:LEU:N	2.17	0.57
1:C:503:ILE:HG22	1:C:512:VAL:HG11	1.85	0.57
1:C:506:ASP:C	1:C:508:PRO:HD3	2.25	0.57
1:D:626:ASP:HB2	1:D:647:LEU:HD12	1.86	0.56
1:A:710:GLU:CG	1:C:559:PRO:HA	2.36	0.56
1:B:548:ILE:HG13	1:B:633:LEU:HD12	1.88	0.56
1:D:596:GLU:O	1:D:597:GLN:HB2	2.05	0.56
1:D:565:GLU:OE1	1:D:641:LYS:HE2	2.05	0.56
1:D:689:PHE:CE2	1:D:693:MET:HE2	2.39	0.56
1:C:463:VAL:O	1:C:466:TYR:HB3	2.06	0.56
1:C:683:GLN:C	1:C:686:VAL:HG12	2.25	0.56
1:C:621:LYS:HB2	1:C:652:ASN:OD1	2.05	0.56
1:A:751:LYS:O	1:A:755:GLU:HG3	2.06	0.56
1:C:580:ARG:HD3	1:C:584:MET:CG	2.32	0.56
1:B:535:MET:HE3	1:B:560:LEU:HD11	1.87	0.55
1:D:535:MET:CE	1:D:560:LEU:HD11	2.36	0.55
1:D:689:PHE:HE2	1:D:693:MET:CE	2.20	0.55
1:C:575:TYR:O	1:C:579:ARG:CD	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:LYS:CG	1:C:715:LEU:N	2.70	0.55
1:D:610:LEU:HD13	1:D:692:LEU:HD21	1.87	0.55
1:A:583:GLY:O	1:A:584:MET:CB	2.54	0.55
1:C:549:ASN:N	1:C:549:ASN:HD22	2.03	0.54
1:C:735:MET:HE2	1:C:753:LEU:HD22	1.88	0.54
1:D:673:GLU:HB3	1:D:679:VAL:CG2	2.38	0.54
1:A:526:LYS:HD3	1:C:662:ASN:HB3	1.89	0.54
1:B:634:VAL:HG23	1:B:638:ASN:HA	1.90	0.54
1:B:759:ARG:HH21	1:B:759:ARG:HB3	1.72	0.54
1:D:548:ILE:HG13	1:D:633:LEU:HD12	1.90	0.54
1:B:630:ARG:HH21	1:B:666:PRO:HG2	1.73	0.54
1:A:549:ASN:ND2	1:A:565:GLU:OE1	2.42	0.53
1:D:503:ILE:HG22	1:D:512:VAL:CG1	2.38	0.53
1:C:683:GLN:CA	1:C:686:VAL:HG12	2.39	0.53
1:D:487:LEU:HD21	1:D:497:MET:HB2	1.91	0.53
1:B:735:MET:HE1	1:B:757:LEU:HD11	1.91	0.53
1:D:536:GLU:OE1	1:D:539:LYS:HD2	2.09	0.53
1:A:575:TYR:O	1:A:579:ARG:CD	2.58	0.52
1:B:693:MET:CE	1:B:736:MET:HA	2.40	0.52
1:A:468:LEU:HD23	1:A:555:THR:HB	1.92	0.52
1:C:683:GLN:O	1:C:686:VAL:CG1	2.58	0.52
1:B:503:ILE:HG22	1:B:512:VAL:CG1	2.40	0.52
1:B:537:MET:O	1:B:541:ILE:HG13	2.10	0.52
1:B:575:TYR:O	1:B:579:ARG:HD2	2.09	0.52
1:A:763:LEU:O	1:A:764:THR:C	2.48	0.51
1:D:486:PRO:HA	1:D:496:VAL:HA	1.92	0.51
1:D:598:MET:HG2	1:D:603:LEU:HD23	1.91	0.51
1:D:658:LYS:NZ	4:D:937:HOH:O	2.40	0.51
1:B:503:ILE:CG2	1:B:512:VAL:HG11	2.41	0.51
1:B:680:TYR:CE2	1:B:684:SER:HB2	2.46	0.51
1:C:610:LEU:HD13	1:C:692:LEU:HD21	1.91	0.50
1:D:477:PRO:HG2	1:D:480:LYS:HG3	1.93	0.50
1:D:528:LEU:O	1:D:532:VAL:HG23	2.12	0.50
1:C:549:ASN:ND2	1:C:549:ASN:H	2.09	0.50
1:B:545:LYS:HD3	1:B:546:ASN:CG	2.32	0.50
1:D:502:GLY:C	1:D:504:ASP:N	2.63	0.50
1:B:495:VAL:HA	1:B:516:VAL:O	2.12	0.49
1:B:625:ARG:HD3	1:B:647:LEU:O	2.12	0.49
1:C:581:PRO:HD2	1:C:584:MET:CE	2.42	0.49
1:C:625:ARG:HG2	1:C:680:TYR:CE2	2.47	0.49
1:B:545:LYS:HZ3	1:B:546:ASN:HD21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:GLU:CG	1:D:597:GLN:N	2.69	0.49
1:A:605:SER:O	1:A:609:GLN:HG3	2.13	0.49
1:B:546:ASN:ND2	1:B:609:GLN:HB3	2.28	0.49
1:D:535:MET:HE1	1:D:560:LEU:HD11	1.94	0.49
1:A:673:GLU:HB3	1:A:679:VAL:HG23	1.93	0.49
1:C:714:LYS:HG3	1:C:715:LEU:N	2.28	0.49
1:D:635:THR:HG23	1:D:636:GLU:HG3	1.93	0.49
1:C:486:PRO:HA	1:C:496:VAL:HA	1.94	0.49
1:A:485:LYS:HB2	1:D:594:PRO:HD3	1.95	0.48
1:C:468:LEU:HD12	1:C:468:LEU:H	1.78	0.48
1:B:466:TYR:C	1:B:467:GLU:HG2	2.33	0.48
1:B:535:MET:HE3	1:B:562:VAL:HG22	1.94	0.48
1:B:708:PRO:HG2	1:B:711:GLU:HG3	1.94	0.48
1:D:598:MET:HG2	1:D:603:LEU:HD21	1.95	0.48
1:D:667:VAL:CG2	1:D:709:VAL:HG22	2.43	0.48
1:B:605:SER:O	1:B:609:GLN:HG3	2.13	0.48
1:D:537:MET:O	1:D:540:MET:HG2	2.14	0.48
1:C:670:MET:HE2	1:C:674:ALA:HB1	1.96	0.48
1:D:595:GLU:O	1:D:596:GLU:O	2.31	0.48
1:A:621:LYS:CD	1:A:652:ASN:ND2	2.77	0.48
1:D:575:TYR:CE1	1:D:579:ARG:NH2	2.82	0.48
1:D:548:ILE:HD13	1:D:641:LYS:HD3	1.96	0.48
1:A:502:GLY:C	1:A:504:ASP:N	2.66	0.48
1:B:506:ASP:C	1:B:508:PRO:HD3	2.34	0.48
1:A:541:ILE:HD13	1:A:617:LEU:HD11	1.95	0.47
1:A:630:ARG:HG2	4:A:912:HOH:O	2.15	0.47
1:B:670:MET:HG2	1:B:674:ALA:HB3	1.97	0.47
1:D:605:SER:O	1:D:609:GLN:HG3	2.14	0.47
1:D:535:MET:HE2	1:D:562:VAL:HG22	1.97	0.47
1:B:687:TRP:CE3	1:B:740:TRP:HA	2.48	0.47
1:D:549:ASN:OD1	1:D:549:ASN:N	2.47	0.47
1:C:468:LEU:HD12	1:C:468:LEU:N	2.29	0.47
1:C:735:MET:CE	1:C:753:LEU:HD22	2.45	0.47
1:B:548:ILE:HD13	1:B:548:ILE:HA	1.86	0.46
1:A:661:THR:CG2	1:C:462:GLY:N	2.78	0.46
1:C:507:LYS:N	1:C:508:PRO:CD	2.78	0.46
1:B:535:MET:HE1	1:B:553:ALA:HB1	1.98	0.46
1:C:584:MET:HG3	1:C:585:GLU:N	2.30	0.46
1:A:556:GLN:O	1:A:557:ASP:C	2.54	0.46
1:A:572:LEU:HD22	1:A:640:MET:HE3	1.98	0.46
1:A:630:ARG:HH21	1:A:666:PRO:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:ARG:HA	1:B:680:TYR:CZ	2.51	0.46
1:D:519:LEU:HD11	1:D:528:LEU:HD13	1.96	0.46
1:D:531:LEU:HD23	1:D:560:LEU:HD23	1.98	0.46
1:B:476:PHE:CD1	1:B:503:ILE:HD12	2.51	0.46
1:B:615:GLU:OE2	1:B:751:LYS:HA	2.15	0.46
1:C:647:LEU:HD13	1:C:665:LEU:HD23	1.98	0.45
1:B:658:LYS:NZ	1:B:678:ARG:HB2	2.32	0.45
1:A:572:LEU:HD13	1:A:640:MET:CE	2.43	0.45
1:A:579:ARG:HG3	1:A:596:GLU:O	2.16	0.45
1:C:463:VAL:HG21	1:C:525:GLU:O	2.15	0.45
1:B:507:LYS:N	1:B:508:PRO:CD	2.79	0.45
1:B:668:LYS:HG2	1:B:712:LEU:HD22	1.97	0.45
1:C:569:LYS:HB2	1:C:634:VAL:HB	1.98	0.45
1:A:759:ARG:O	1:A:763:LEU:HG	2.17	0.45
1:C:466:TYR:C	1:C:467:GLU:HG2	2.37	0.45
1:D:697:PHE:CZ	1:D:732:LEU:HD13	2.51	0.45
1:A:604:VAL:HG12	1:A:761:LEU:HD13	1.99	0.45
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.99	0.45
1:B:600:PHE:CZ	1:B:729:THR:HG23	2.52	0.45
1:D:544:HIS:HE1	1:D:546:ASN:HD22	1.65	0.45
1:B:617:LEU:HG	1:B:622:CYS:O	2.17	0.45
1:C:680:TYR:CE2	1:C:684:SER:HB2	2.52	0.45
1:B:677:ASP:O	1:B:679:VAL:HG13	2.18	0.44
1:B:759:ARG:CB	1:B:759:ARG:HH21	2.30	0.44
1:B:670:MET:SD	1:B:675:LEU:HG	2.57	0.44
1:B:756:ASP:HA	1:B:759:ARG:HH22	1.82	0.44
1:C:504:ASP:OD1	1:C:506:ASP:HB2	2.17	0.44
1:B:545:LYS:HD3	1:B:546:ASN:ND2	2.33	0.43
1:A:652:ASN:O	1:A:653:ASN:HB2	2.18	0.43
1:D:467:GLU:CG	1:D:468:LEU:N	2.81	0.43
1:A:528:LEU:O	1:A:532:VAL:HG23	2.18	0.43
1:D:580:ARG:HA	1:D:581:PRO:HD3	1.84	0.43
1:A:525:GLU:CD	1:C:675:LEU:HD11	2.38	0.43
1:A:750:PHE:O	1:A:754:VAL:HG23	2.18	0.43
1:B:678:ARG:HH22	1:D:525:GLU:CD	2.22	0.43
1:A:548:ILE:HD13	1:A:548:ILE:HA	1.92	0.43
1:A:571:ASN:HD21	1:A:574:GLU:CD	2.21	0.43
1:A:594:PRO:C	1:A:596:GLU:H	2.22	0.43
1:A:659:ASN:O	1:A:678:ARG:HD2	2.18	0.43
1:C:708:PRO:HG2	1:C:711:GLU:HG3	1.99	0.43
1:D:502:GLY:C	1:D:504:ASP:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:ALA:HB1	1:B:673:GLU:OE2	2.19	0.43
1:C:468:LEU:H	1:C:468:LEU:CD1	2.32	0.43
1:D:548:ILE:HA	1:D:548:ILE:HD13	1.85	0.43
1:B:647:LEU:HD13	1:B:665:LEU:HD23	2.00	0.42
1:B:651:ILE:O	1:B:652:ASN:C	2.57	0.42
1:C:714:LYS:CG	1:C:715:LEU:H	2.32	0.42
1:A:660:THR:HG23	2:A:801:SO4:O1	2.20	0.42
1:B:693:MET:HE1	1:B:736:MET:HA	2.01	0.42
1:A:595:GLU:CD	1:D:636:GLU:HB3	2.40	0.42
1:A:477:PRO:HB2	1:A:479:ASP:OD1	2.20	0.42
1:D:535:MET:HE3	1:D:560:LEU:HD11	2.00	0.42
1:C:673:GLU:CD	1:C:673:GLU:H	2.22	0.42
1:D:693:MET:HE1	1:D:735:MET:SD	2.59	0.42
1:B:549:ASN:ND2	4:B:9014:HOH:O	2.53	0.41
1:D:593:VAL:HA	1:D:594:PRO:HD2	1.95	0.41
1:C:545:LYS:HG2	1:C:545:LYS:O	2.20	0.41
1:B:589:ASP:CB	1:C:485:LYS:NZ	2.83	0.41
1:B:545:LYS:HZ2	1:B:546:ASN:HD21	1.69	0.41
1:A:600:PHE:CZ	1:A:729:THR:HG23	2.56	0.41
1:D:652:ASN:O	1:D:653:ASN:HB2	2.20	0.41
1:B:714:LYS:HG2	1:B:718:GLU:OE2	2.19	0.41
1:C:698:THR:HG22	1:C:725:PRO:HB3	2.02	0.41
1:A:708:PRO:HG2	1:A:711:GLU:HG3	2.03	0.41
1:B:571:ASN:HA	1:B:632:VAL:O	2.21	0.41
1:D:621:LYS:HD3	1:D:652:ASN:HA	2.03	0.41
1:A:549:ASN:ND2	1:A:549:ASN:N	2.46	0.40
1:B:678:ARG:NH2	1:D:525:GLU:OE2	2.49	0.40
1:A:621:LYS:HD3	1:A:652:ASN:HD22	1.86	0.40
1:B:673:GLU:CD	1:B:673:GLU:H	2.23	0.40
1:C:581:PRO:HD2	1:C:584:MET:HE2	2.03	0.40
1:C:605:SER:O	1:C:609:GLN:HG3	2.20	0.40
1:D:617:LEU:HA	1:D:617:LEU:HD12	1.90	0.40
1:D:738:ASP:HB3	1:D:748:PRO:HD3	2.03	0.40
1:A:506:ASP:C	1:A:508:PRO:HD3	2.41	0.40
1:A:540:MET:HE1	1:A:622:CYS:SG	2.61	0.40
1:A:637:ASN:OD1	1:A:637:ASN:N	2.54	0.40
1:C:612:ARG:HG2	1:C:612:ARG:HH11	1.86	0.40
1:D:750:PHE:O	1:D:754:VAL:HG23	2.21	0.40
1:A:596:GLU:O	1:A:597:GLN:C	2.60	0.40
1:A:658:LYS:NZ	4:A:944:HOH:O	2.55	0.40
1:D:581:PRO:HA	1:D:582:PRO:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:749:THR:OG1	1:D:752:GLN:HG3	2.21	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	282/324 (87%)	264 (94%)	14 (5%)	4 (1%)	14	10
1	B	276/324 (85%)	262 (95%)	11 (4%)	3 (1%)	17	14
1	C	275/324 (85%)	257 (94%)	15 (6%)	3 (1%)	17	14
1	D	277/324 (86%)	263 (95%)	10 (4%)	4 (1%)	14	10
All	All	1110/1296 (86%)	1046 (94%)	50 (4%)	14 (1%)	15	11

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	ILE
1	A	636	GLU
1	A	763	LEU
1	D	468	LEU
1	D	596	GLU
1	C	464	SER
1	D	636	GLU
1	A	557	ASP
1	B	464	SER
1	B	652	ASN
1	C	557	ASP
1	D	508	PRO
1	C	644	ASP
1	B	590	ILE

5.3.2 Protein sidechains ⓘ

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	246/284 (87%)	238 (97%)	8 (3%)	45	56
1	B	247/284 (87%)	237 (96%)	10 (4%)	38	47
1	C	247/284 (87%)	241 (98%)	6 (2%)	57	69
1	D	244/284 (86%)	236 (97%)	8 (3%)	45	56
All	All	984/1136 (87%)	952 (97%)	32 (3%)	45	56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	548	ILE
1	A	549	ASN
1	A	579	ARG
1	A	598	MET
1	A	606	CYS
1	A	636	GLU
1	A	637	ASN
1	A	723	ASP
1	B	467	GLU
1	B	479	ASP
1	B	548	ILE
1	B	573	ARG
1	B	579	ARG
1	B	622	CYS
1	B	634	VAL
1	B	673	GLU
1	B	675	LEU
1	B	723	ASP
1	C	549	ASN
1	C	579	ARG
1	C	598	MET
1	C	637	ASN
1	C	673	GLU
1	C	730	ASN

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Mol	Chain	Res	Type
1	D	468	LEU
1	D	512	VAL
1	D	548	ILE
1	D	595	GLU
1	D	598	MET
1	D	622	CYS
1	D	636	GLU
1	D	644	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	ASN
1	A	631	ASN
1	A	652	ASN
1	A	653	ASN
1	A	683	GLN
1	B	546	ASN
1	B	549	ASN
1	B	631	ASN
1	C	549	ASN
1	C	597	GLN
1	C	631	ASN
1	C	637	ASN
1	C	638	ASN
1	C	653	ASN
1	C	662	ASN
1	C	746	GLN
1	D	546	ASN
1	D	597	GLN
1	D	631	ASN
1	D	653	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	SO4	A	801	-	4,4,4	0.18	0	6,6,6	0.11	0
3	ACP	A	802	-	16,19,33	0.56	0	14,28,52	0.61	0
2	SO4	B	8001	-	4,4,4	0.16	0	6,6,6	0.06	0
3	ACP	B	8002	-	29,33,33	2.83	6 (20%)	29,52,52	1.13	3 (10%)
2	SO4	C	801	-	4,4,4	0.16	0	6,6,6	0.07	0
3	ACP	C	802	-	16,19,33	0.60	0	14,28,52	0.72	0
2	SO4	D	801	-	4,4,4	0.25	0	6,6,6	0.09	0
3	ACP	D	802	-	16,19,33	0.57	0	14,28,52	0.69	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
2	SO4	A	801	-	-	0/0/0/0	0/0/0/0
3	ACP	A	802	-	-	0/0/17/38	0/3/3/3
2	SO4	B	8001	-	-	0/0/0/0	0/0/0/0
3	ACP	B	8002	-	-	0/15/38/38	0/3/3/3
2	SO4	C	801	-	-	0/0/0/0	0/0/0/0
3	ACP	C	802	-	-	0/0/17/38	0/3/3/3
2	SO4	D	801	-	-	0/0/0/0	0/0/0/0
3	ACP	D	802	-	-	0/0/17/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	8002	ACP	PG-C3B	-9.85	1.70	1.80
3	B	8002	ACP	PB-C3B	-9.80	1.70	1.80
3	B	8002	ACP	PB-O3A	-3.78	1.54	1.58
3	B	8002	ACP	PB-O2B	-2.55	1.50	1.56
3	B	8002	ACP	PG-O2G	-2.23	1.49	1.54
3	B	8002	ACP	PG-O3G	-2.16	1.49	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	8002	ACP	O1G-PG-C3B	-3.61	102.86	111.37
3	B	8002	ACP	O3G-PG-O2G	2.16	114.67	108.12
3	B	8002	ACP	O2B-PB-O1B	2.39	117.87	110.24

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
2	A	801	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, 95th 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	288/324 (88%)	-0.11	6 (2%) 67 65	19, 30, 50, 61	0
1	B	286/324 (88%)	-0.03	6 (2%) 67 65	19, 34, 55, 86	0
1	C	285/324 (87%)	0.08	11 (3%) 43 42	20, 35, 59, 79	0
1	D	283/324 (87%)	-0.11	5 (1%) 71 70	16, 29, 48, 64	0
All	All	1142/1296 (88%)	-0.04	28 (2%) 61 60	16, 32, 54, 86	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	TYR	5.6
1	D	467	GLU	4.2
1	C	466	TYR	4.1
1	C	584	MET	3.6
1	B	656	TYR	3.4
1	D	506	ASP	3.2
1	D	505	LYS	3.1
1	B	727	ASN	3.0
1	B	467	GLU	3.0
1	C	656	TYR	2.9
1	C	510	GLU	2.9
1	C	653	ASN	2.8
1	A	635	THR	2.6
1	A	727	ASN	2.6
1	D	508	PRO	2.5
1	A	637	ASN	2.5
1	C	657	TYR	2.5
1	A	583	GLY	2.3
1	B	462	GLY	2.3
1	A	506	ASP	2.3
1	C	462	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	636	GLU	2.2
1	C	506	ASP	2.1
1	A	636	GLU	2.1
1	C	675	LEU	2.1
1	C	728	CYS	2.1
1	C	467	GLU	2.1
1	B	653	ASN	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, 95th 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	ACP	B	8002	31/31	0.85	0.19	3.30	38,58,85,85	0
3	ACP	A	802	17/31	0.83	0.20	3.29	42,44,51,53	0
2	SO4	A	801	5/5	0.90	0.18	1.77	78,79,79,79	0
3	ACP	D	802	17/31	0.89	0.16	0.68	33,39,50,54	0
3	ACP	C	802	17/31	0.92	0.14	0.26	33,36,44,46	0
2	SO4	B	8001	5/5	0.97	0.12	-0.56	62,62,63,63	0
2	SO4	D	801	5/5	0.95	0.12	-0.97	54,54,55,55	0
2	SO4	C	801	5/5	0.95	0.16	-	62,62,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.