



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 01:20 pm GMT

PDB ID : 4Z3L
Title : CRYSTAL STRUCTURE OF BIRCH POLLEN ALLERGEN BET V 1 MUTANT G26L, D69I, P90L, K97I
Authors : Freier, R.; Brandstetter, H.
Deposited on : 2015-03-31
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

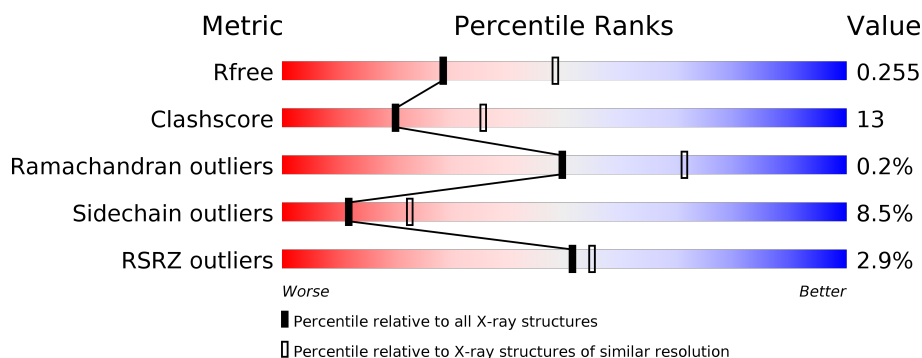
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (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 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	159	<div> <div>77%</div> <div>17%</div> <div>5%</div> <div>•</div> </div>
1	B	159	<div> <div>79%</div> <div>18%</div> <div>•</div> </div>
1	C	159	<div> <div>3%</div> <div>69%</div> <div>26%</div> <div>•</div> </div>
1	D	159	<div> <div>5%</div> <div>72%</div> <div>19%</div> <div>8%</div> </div>
1	E	159	<div> <div>4%</div> <div>73%</div> <div>22%</div> <div>• •</div> </div>
1	F	159	<div> <div>3%</div> <div>76%</div> <div>20%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	202	-	-	X	-
2	SO4	E	201	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7745 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 Major pollen allergen Bet v 1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	1	0
			1240	795	201	243	1			
1	B	159	Total	C	N	O	S	0	1	0
			1240	795	201	243	1			
1	C	159	Total	C	N	O	S	0	2	0
			1254	809	201	243	1			
1	E	159	Total	C	N	O	S	0	0	0
			1233	790	200	242	1			
1	F	159	Total	C	N	O	S	0	1	0
			1242	796	202	243	1			
1	D	159	Total	C	N	O	S	0	1	0
			1246	801	201	243	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	LEU	GLY	engineered mutation	UNP P15494
A	69	ILE	ASP	engineered mutation	UNP P15494
A	90	LEU	PRO	engineered mutation	UNP P15494
A	97	ILE	LYS	engineered mutation	UNP P15494
B	26	LEU	GLY	engineered mutation	UNP P15494
B	69	ILE	ASP	engineered mutation	UNP P15494
B	90	LEU	PRO	engineered mutation	UNP P15494
B	97	ILE	LYS	engineered mutation	UNP P15494
C	26	LEU	GLY	engineered mutation	UNP P15494
C	69	ILE	ASP	engineered mutation	UNP P15494
C	90	LEU	PRO	engineered mutation	UNP P15494
C	97	ILE	LYS	engineered mutation	UNP P15494
E	26	LEU	GLY	engineered mutation	UNP P15494
E	69	ILE	ASP	engineered mutation	UNP P15494
E	90	LEU	PRO	engineered mutation	UNP P15494
E	97	ILE	LYS	engineered mutation	UNP P15494
F	26	LEU	GLY	engineered mutation	UNP P15494

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Chain	Residue	Modelled	Actual	Comment	Reference
F	69	ILE	ASP	engineered mutation	UNP P15494
F	90	LEU	PRO	engineered mutation	UNP P15494
F	97	ILE	LYS	engineered mutation	UNP P15494
D	26	LEU	GLY	engineered mutation	UNP P15494
D	69	ILE	ASP	engineered mutation	UNP P15494
D	90	LEU	PRO	engineered mutation	UNP P15494
D	97	ILE	LYS	engineered mutation	UNP P15494

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	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		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

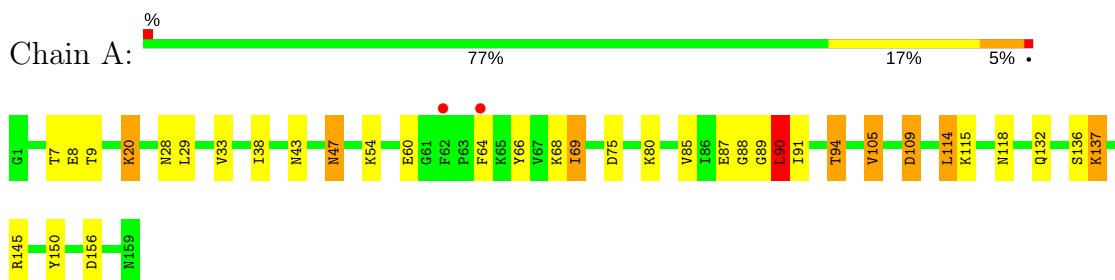
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	47	Total O 47 47	0	0
3	B	49	Total O 49 49	0	0
3	C	32	Total O 32 32	0	0
3	E	29	Total O 29 29	0	0
3	F	37	Total O 37 37	0	0
3	D	26	Total O 26 26	0	0

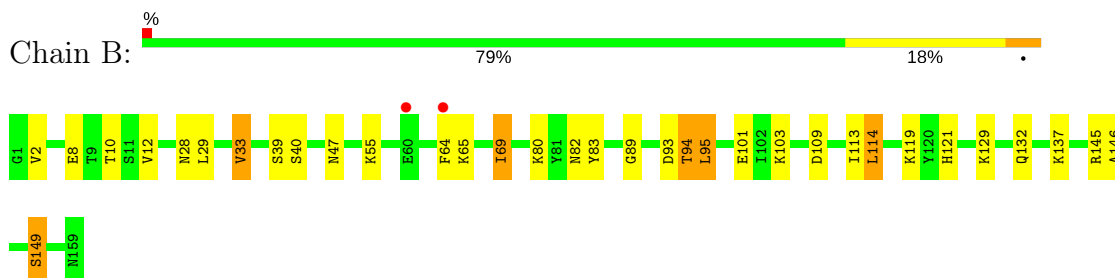
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

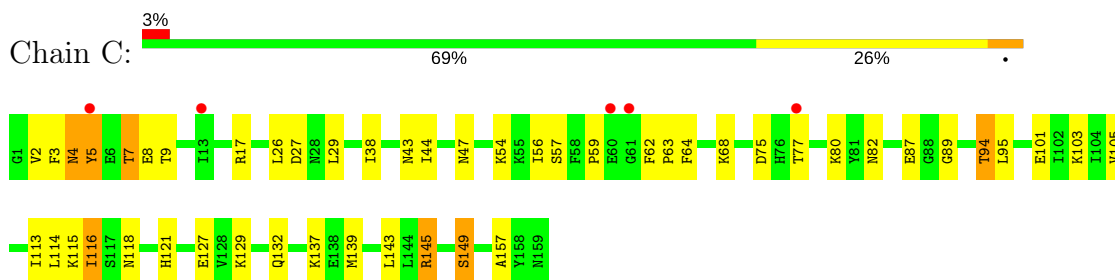
- Molecule 1: Major pollen allergen Bet v 1-A



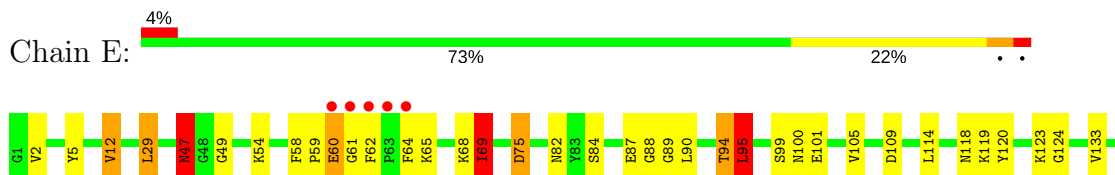
- Molecule 1: Major pollen allergen Bet v 1-A

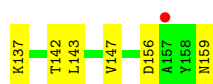


- Molecule 1: Major pollen allergen Bet v 1-A

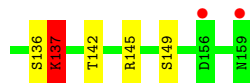
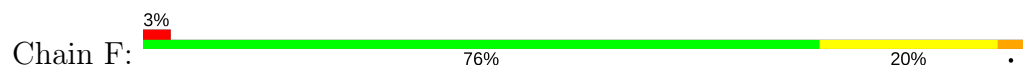


- Molecule 1: Major pollen allergen Bet v 1-A

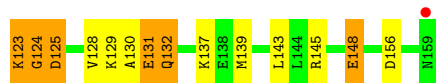
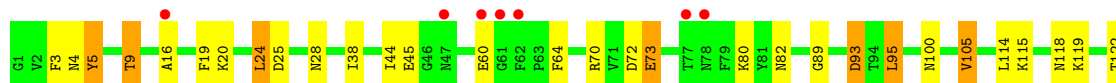
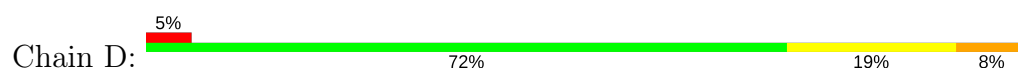




- Molecule 1: Major pollen allergen Bet v 1-A



- Molecule 1: Major pollen allergen Bet v 1-A



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.29Å 143.34Å 148.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.02 – 2.50 37.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.02-2.50) 99.6 (37.02-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.212 , 0.256 0.212 , 0.255	Depositor DCC
R_{free} test set	2330 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7745	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7279e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	1.07	0/1268	1.13	8/1714 (0.5%)
1	B	1.07	1/1268 (0.1%)	1.12	3/1714 (0.2%)
1	C	1.08	3/1287 (0.2%)	1.19	6/1740 (0.3%)
1	D	1.10	1/1275 (0.1%)	1.18	7/1724 (0.4%)
1	E	1.05	1/1258 (0.1%)	1.17	6/1702 (0.4%)
1	F	1.03	0/1270	1.11	6/1717 (0.3%)
All	All	1.07	6/7626 (0.1%)	1.15	36/10311 (0.3%)

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	D	0	1
1	E	0	2
1	F	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	ASN	C-N	7.29	1.50	1.34
1	E	69	ILE	C-N	-6.53	1.19	1.34
1	D	73	GLU	CG-CD	6.38	1.61	1.51
1	B	47	ASN	CB-CG	5.05	1.62	1.51
1	C	5[A]	TYR	C-N	-5.01	1.22	1.34
1	C	5[B]	TYR	C-N	-5.01	1.22	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	ASN	O-C-N	-10.81	105.40	122.70
1	E	69	ILE	O-C-N	-8.92	108.42	122.70
1	D	80	LYS	CD-CE-NZ	-8.74	91.60	111.70
1	C	5[A]	TYR	C-N-CA	-8.37	100.77	121.70
1	C	5[B]	TYR	C-N-CA	-8.37	100.77	121.70
1	B	114	LEU	CB-CG-CD1	-7.88	97.60	111.00
1	A	114	LEU	CB-CG-CD1	-7.49	98.27	111.00
1	F	72	ASP	CB-CG-OD1	7.38	124.94	118.30
1	F	145	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	5[A]	TYR	O-C-N	6.63	133.31	122.70
1	C	5[B]	TYR	O-C-N	6.63	133.31	122.70
1	F	72	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	E	143	LEU	CB-CG-CD1	-6.52	99.92	111.00
1	D	95	LEU	CA-CB-CG	6.35	129.91	115.30
1	D	73	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	D	93	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	70	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	93	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	90	LEU	CA-CB-CG	5.74	128.50	115.30
1	E	95	LEU	CA-CB-CG	5.69	128.40	115.30
1	C	75	ASP	CB-CG-OD1	5.67	123.40	118.30
1	F	62	PHE	C-N-CD	5.64	140.25	128.40
1	A	156	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	E	124	GLY	N-CA-C	-5.51	99.33	113.10
1	A	145	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	109	ASP	CB-CA-C	-5.46	99.48	110.40
1	B	114	LEU	CB-CA-C	-5.31	100.11	110.20
1	F	137	LYS	CD-CE-NZ	5.31	123.90	111.70
1	A	145	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	58	PHE	C-N-CD	5.26	139.44	128.40
1	A	20	LYS	CD-CE-NZ	-5.21	99.72	111.70
1	E	75	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	D	5[A]	TYR	O-C-N	-5.12	114.51	122.70
1	D	5[B]	TYR	O-C-N	-5.12	114.51	122.70
1	A	156	ASP	CB-CG-OD1	5.10	122.89	118.30
1	E	12	VAL	CG1-CB-CG2	5.07	119.01	110.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	123	LYS	Peptide
1	E	47	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	69	ILE	Mainchain
1	F	59	PRO	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	A	1240	0	1241	38	0
1	B	1240	0	1241	27	0
1	C	1254	0	1254	60	0
1	D	1246	0	1242	43	0
1	E	1233	0	1224	36	0
1	F	1242	0	1242	20	0
2	A	15	0	0	0	0
2	B	20	0	0	2	0
2	C	5	0	0	1	0
2	E	5	0	0	0	2
2	F	25	0	0	2	0
3	A	47	0	0	3	0
3	B	49	0	0	3	1
3	C	32	0	0	3	0
3	D	26	0	0	0	0
3	E	29	0	0	0	0
3	F	37	0	0	1	1
All	All	7745	0	7444	202	3

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 13.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3[B]:PHE:CE1	1:D:128:VAL:HG21	1.23	1.62
1:C:3[B]:PHE:CE1	1:D:128:VAL:CG2	1.96	1.47
1:E:47:ASN:HB2	1:E:49:GLY:H	1.07	1.11
1:C:3[B]:PHE:CZ	1:D:122:THR:HG23	1.89	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3[B]:PHE:HE1	1:D:128:VAL:CG2	1.50	0.99
1:C:17:ARG:NH1	1:C:157:ALA:O	1.97	0.96
1:A:90:LEU:HD23	1:A:132:GLN:NE2	1.80	0.96
1:C:59:PRO:HD2	1:C:62:PHE:CE1	2.02	0.94
1:C:3[B]:PHE:CD1	1:D:128:VAL:CG2	2.52	0.92
1:C:80:LYS:HE2	1:C:103:LYS:HE3	1.49	0.92
1:B:114:LEU:N	1:B:114:LEU:HD12	1.83	0.92
1:C:3[B]:PHE:CE1	1:D:128:VAL:HG23	2.05	0.90
1:D:38:ILE:HD12	1:D:143:LEU:HD21	1.55	0.89
1:A:105:VAL:HG21	1:A:115:LYS:HE3	1.55	0.89
1:C:3[B]:PHE:CD1	1:D:128:VAL:HG21	2.06	0.89
1:D:123:LYS:O	1:D:124:GLY:O	1.90	0.88
1:C:3[B]:PHE:CD1	1:D:128:VAL:HB	2.08	0.88
1:B:129:LYS:H	1:B:132:GLN:HE21	1.17	0.88
1:B:82:ASN:OD1	1:B:101:GLU:HG3	1.73	0.88
1:B:33:VAL:HG13	1:B:146:ALA:HB1	1.57	0.87
3:C:301:HOH:O	1:D:4:ASN:HB2	1.74	0.87
1:C:3[B]:PHE:HZ	1:D:122:THR:HG23	1.41	0.85
1:A:90:LEU:HB3	1:A:94:THR:HG22	1.56	0.84
1:C:3[B]:PHE:CZ	1:D:122:THR:CG2	2.63	0.82
1:F:53:ILE:HG21	2:F:205:SO4:O2	1.79	0.81
1:B:65:LYS:O	1:B:65:LYS:HD2	1.82	0.79
1:C:3[A]:PHE:HE2	1:C:5[A]:TYR:CD1	1.99	0.79
1:A:90:LEU:HD23	1:A:132:GLN:HE21	1.48	0.78
1:E:5:TYR:OH	1:E:137:LYS:HE2	1.84	0.78
1:A:69:ILE:HD11	1:A:85:VAL:HG22	1.64	0.77
1:C:3[B]:PHE:CD1	1:D:128:VAL:CB	2.66	0.77
1:C:3[B]:PHE:HD1	1:D:128:VAL:HB	1.49	0.77
2:B:202:SO4:O3	1:E:133:VAL:HG11	1.86	0.76
1:C:94:THR:HG22	1:C:95:LEU:HG	1.68	0.75
1:F:80:LYS:HG3	1:F:103:LYS:HG3	1.67	0.75
1:C:3[B]:PHE:CD2	1:D:3:PHE:CD2	2.64	0.75
1:E:59:PRO:HG2	1:E:62:PHE:CD2	2.22	0.75
1:A:69:ILE:CD1	1:A:85:VAL:HG22	2.17	0.75
1:D:5[B]:TYR:OH	1:D:137:LYS:HD2	1.88	0.73
1:E:47:ASN:HB2	1:E:49:GLY:N	1.93	0.72
1:C:59:PRO:HD2	1:C:62:PHE:HE1	1.54	0.72
1:C:3[A]:PHE:HE2	1:C:5[A]:TYR:CE1	2.07	0.72
1:C:3[A]:PHE:CE2	1:C:5[A]:TYR:CE1	2.78	0.71
1:B:69:ILE:HG12	1:B:83:TYR:HD2	1.57	0.70
1:A:118:ASN:ND2	3:A:301:HOH:O	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ASN:OD1	1:C:101:GLU:HG3	1.94	0.67
1:B:69:ILE:HG12	1:B:83:TYR:CD2	2.29	0.67
1:E:59:PRO:HD2	1:E:62:PHE:HD2	1.60	0.67
1:C:3[A]:PHE:HD2	1:C:5[A]:TYR:CE2	2.13	0.67
1:A:47:ASN:N	1:A:47:ASN:OD1	2.27	0.66
1:B:137:LYS:HE2	3:B:335:HOH:O	1.95	0.66
1:B:94:THR:HG22	1:B:95:LEU:HD13	1.78	0.65
1:E:90:LEU:HD13	1:E:94:THR:HG21	1.79	0.65
1:C:3[A]:PHE:CD2	1:C:5[A]:TYR:CE2	2.85	0.65
1:E:94:THR:HG23	1:E:95:LEU:HD13	1.79	0.65
1:C:38:ILE:HD12	1:C:143:LEU:HD21	1.79	0.64
1:E:59:PRO:HD2	1:E:62:PHE:CD2	2.32	0.64
1:A:7:THR:HG23	1:A:137:LYS:HE2	1.80	0.64
1:B:114:LEU:N	1:B:114:LEU:CD1	2.60	0.64
1:B:55:LYS:NZ	3:B:301:HOH:O	2.22	0.64
1:C:59:PRO:HD2	1:C:62:PHE:CD1	2.33	0.64
1:F:94:THR:HG22	1:F:95:LEU:HG	1.79	0.64
1:C:127:GLU:OE2	3:C:301:HOH:O	2.15	0.64
1:B:121:HIS:HD2	1:C:121:HIS:HD2	1.47	0.63
1:C:27:ASP:OD1	1:C:54:LYS:HE2	1.99	0.63
1:A:88:GLY:O	1:A:91:ILE:HG12	1.98	0.63
1:E:54:LYS:HD2	1:E:69:ILE:HD11	1.81	0.63
1:B:114:LEU:H	1:B:114:LEU:HD12	1.60	0.62
1:C:129:LYS:O	1:C:132:GLN:HG2	1.99	0.62
1:D:25:ASP:OD1	1:D:28:ASN:ND2	2.29	0.61
1:A:64:PHE:CD1	1:A:89:GLY:HA2	2.34	0.61
1:B:33:VAL:HG13	1:B:146:ALA:CB	2.27	0.61
1:A:7:THR:HG22	3:A:311:HOH:O	2.01	0.61
1:B:137:LYS:CE	3:B:335:HOH:O	2.49	0.60
1:E:60:GLU:H	1:E:60:GLU:CD	2.05	0.60
1:C:7:THR:HG22	1:C:116:ILE:HG23	1.82	0.60
1:E:59:PRO:HG2	1:E:62:PHE:HD2	1.64	0.59
2:B:202:SO4:O3	1:E:133:VAL:CG1	2.50	0.59
1:E:68:LYS:NZ	1:F:45:GLU:OE2	2.36	0.59
1:C:80:LYS:HE2	1:C:103:LYS:CE	2.27	0.59
1:E:59:PRO:CD	1:E:62:PHE:HD2	2.16	0.58
1:E:156:ASP:HA	1:E:159:ASN:ND2	2.19	0.57
1:A:114:LEU:HD12	1:A:114:LEU:N	2.19	0.57
1:E:64:PHE:CD1	1:E:89:GLY:HA2	2.40	0.57
1:E:59:PRO:CG	1:E:62:PHE:CD2	2.87	0.57
1:E:2:VAL:HA	1:E:120:TYR:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LYS:H	1:C:132:GLN:NE2	2.03	0.56
1:C:3[A]:PHE:CE2	1:C:5[A]:TYR:CZ	2.93	0.56
1:A:43:ASN:OD1	1:A:54:LYS:HE2	2.05	0.56
1:A:20:LYS:HE2	3:A:323:HOH:O	2.06	0.56
1:B:80:LYS:HG3	1:B:103:LYS:HD2	1.89	0.55
1:C:3[B]:PHE:CE2	1:D:122:THR:HG23	2.38	0.55
1:C:43:ASN:OD1	1:C:54:LYS:HE3	2.06	0.55
1:E:59:PRO:CG	1:E:62:PHE:HD2	2.20	0.54
1:C:116:ILE:CD1	1:C:118:ASN:HD21	2.20	0.54
1:C:105:VAL:HG22	1:C:113:ILE:CG2	2.37	0.54
1:D:38:ILE:CD1	1:D:143:LEU:HD21	2.34	0.54
1:E:64:PHE:CG	1:E:89:GLY:HA2	2.43	0.54
1:C:68:LYS:HD2	1:C:87:GLU:OE1	2.08	0.53
1:A:90:LEU:CD2	1:A:132:GLN:HE21	2.19	0.53
1:A:90:LEU:CD2	1:A:132:GLN:NE2	2.62	0.53
1:C:116:ILE:HD11	1:C:118:ASN:HD21	1.74	0.53
1:C:26:LEU:HD22	2:C:201:SO4:O2	2.09	0.53
1:E:2:VAL:HG23	1:E:2:VAL:O	2.07	0.52
1:C:7:THR:CG2	1:C:116:ILE:HG23	2.39	0.52
1:D:123:LYS:O	1:D:124:GLY:C	2.48	0.52
1:E:100:ASN:HD22	1:E:118:ASN:HA	1.75	0.52
1:E:69:ILE:HA	1:E:84:SER:O	2.09	0.51
1:A:66:TYR:C	1:A:66:TYR:CD1	2.84	0.51
1:A:90:LEU:HD23	1:A:132:GLN:HE22	1.66	0.51
1:A:7:THR:CG2	1:A:137:LYS:HE2	2.40	0.51
1:A:90:LEU:HB3	1:A:94:THR:CG2	2.36	0.51
1:B:114:LEU:H	1:B:114:LEU:CD1	2.23	0.51
1:C:3[B]:PHE:HD1	1:D:128:VAL:CB	2.16	0.50
1:C:56:ILE:N	1:C:56:ILE:HD12	2.26	0.49
1:C:3[A]:PHE:CD2	1:C:5[A]:TYR:CZ	3.00	0.49
1:D:72:ASP:O	1:D:73:GLU:HG3	2.12	0.49
1:A:28:ASN:ND2	1:B:28:ASN:HB3	2.28	0.49
1:E:87:GLU:HG2	1:E:88:GLY:N	2.26	0.49
1:A:105:VAL:CG2	1:A:115:LYS:HE3	2.33	0.49
1:F:90:LEU:HB3	1:F:94:THR:HG22	1.93	0.49
1:C:62:PHE:HB3	1:C:63:PRO:CD	2.43	0.49
1:B:10:THR:HG22	1:B:113:ILE:HG12	1.95	0.49
1:D:9:THR:HG23	1:D:114:LEU:HB2	1.95	0.49
1:B:2:VAL:HB	1:D:125:ASP:HB2	1.95	0.48
1:B:29:LEU:O	1:B:33:VAL:HB	2.13	0.48
1:B:121:HIS:CD2	1:C:121:HIS:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:HD12	1:A:85:VAL:HA	1.96	0.47
1:C:105:VAL:HG22	1:C:113:ILE:HG23	1.96	0.47
1:F:5:TYR:HE1	1:F:137:LYS:HZ2	1.62	0.47
1:B:8:GLU:HA	1:B:114:LEU:O	2.15	0.47
1:E:90:LEU:HB3	1:E:94:THR:HG22	1.97	0.47
1:C:80:LYS:HG2	1:C:103:LYS:HG3	1.97	0.47
1:E:5:TYR:OH	1:E:137:LYS:CE	2.59	0.47
1:F:70:ARG:HB2	1:F:86:ILE:HD13	1.96	0.46
1:B:64:PHE:CG	1:B:89:GLY:HA2	2.50	0.46
1:C:64:PHE:CD1	1:C:89:GLY:HA2	2.50	0.46
1:C:4:ASN:ND2	1:D:130:ALA:HB2	2.30	0.46
1:F:93:ASP:HA	3:F:316:HOH:O	2.14	0.46
1:D:44:ILE:HG22	1:D:45:GLU:HG3	1.96	0.46
1:E:47:ASN:N	1:E:47:ASN:OD1	2.49	0.46
1:F:3:PHE:CE2	1:F:5:TYR:HB2	2.50	0.46
1:D:16:ALA:O	1:D:20:LYS:HG3	2.16	0.46
1:D:105:VAL:CG1	1:D:115:LYS:HE2	2.46	0.45
1:F:5:TYR:OH	1:F:137:LYS:HE3	2.15	0.45
1:E:82:ASN:ND2	1:E:101:GLU:HG3	2.31	0.45
1:F:2:VAL:HA	1:F:120:TYR:O	2.17	0.45
1:D:5[B]:TYR:HD2	1:D:118:ASN:HD22	1.63	0.45
1:A:43:ASN:OD1	1:A:54:LYS:CE	2.65	0.45
1:D:131:GLU:H	1:D:131:GLU:CD	2.20	0.45
1:F:90:LEU:HD12	1:F:132:GLN:HE22	1.82	0.45
1:A:29:LEU:O	1:A:33:VAL:HG22	2.17	0.44
1:C:8:GLU:OE2	1:C:115:LYS:HG2	2.17	0.44
1:D:73:GLU:HB2	1:D:82:ASN:HB2	1.99	0.44
1:C:145:ARG:O	1:C:149:SER:HB3	2.17	0.44
1:F:59:PRO:HG2	1:F:62:PHE:CD2	2.53	0.44
1:C:105:VAL:CG2	1:C:113:ILE:HG22	2.48	0.43
1:E:114:LEU:N	1:E:114:LEU:HD12	2.32	0.43
1:C:105:VAL:CG2	1:C:113:ILE:CG2	2.96	0.43
1:A:66:TYR:OH	1:A:87:GLU:OE2	2.30	0.43
1:A:64:PHE:CG	1:A:89:GLY:HA2	2.53	0.43
1:D:19:PHE:CE2	1:D:24:LEU:HD13	2.54	0.43
1:A:60:GLU:H	1:A:60:GLU:CD	2.22	0.43
1:A:68:LYS:HB2	1:A:87:GLU:HB3	2.00	0.43
1:A:75:ASP:HB3	1:A:80:LYS:HB2	2.01	0.43
1:B:145:ARG:O	1:B:149:SER:HB3	2.19	0.43
1:A:109:ASP:OD1	1:A:109:ASP:N	2.51	0.43
1:B:64:PHE:CD1	1:B:89:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:VAL:HG11	1:D:115:LYS:HE2	2.00	0.43
1:A:69:ILE:HD12	1:A:85:VAL:HG22	1.99	0.42
1:B:39:SER:O	1:B:40:SER:HB3	2.18	0.42
1:C:3[A]:PHE:CE2	1:C:5[A]:TYR:CD1	2.91	0.42
1:C:3[B]:PHE:HE1	1:D:128:VAL:HG21	0.55	0.42
1:D:100:ASN:HD22	1:D:118:ASN:HA	1.83	0.42
1:C:145:ARG:HA	1:C:145:ARG:HD3	1.75	0.42
1:C:29:LEU:HD23	1:C:29:LEU:HA	1.81	0.42
1:E:29:LEU:HD13	1:E:147:VAL:HG22	2.01	0.42
1:A:87:GLU:HG2	1:A:88:GLY:N	2.34	0.41
1:D:64:PHE:CD1	1:D:89:GLY:HA2	2.55	0.41
1:E:75:ASP:C	1:E:75:ASP:OD1	2.59	0.41
1:A:150:TYR:CD1	1:A:150:TYR:C	2.93	0.41
1:E:59:PRO:C	1:E:61:GLY:N	2.73	0.41
1:E:59:PRO:O	1:E:61:GLY:N	2.53	0.41
1:F:32:LYS:HE2	1:F:32:LYS:HB2	1.95	0.41
1:F:104:ILE:HG21	1:F:104:ILE:HD13	1.78	0.41
1:F:94:THR:CG2	1:F:95:LEU:HG	2.47	0.41
1:D:3:PHE:CD1	1:D:3:PHE:N	2.88	0.41
1:A:80:LYS:HE2	1:A:80:LYS:HB3	1.85	0.41
3:C:301:HOH:O	1:D:4:ASN:CB	2.51	0.41
1:F:100:ASN:OD1	1:F:118:ASN:ND2	2.53	0.41
1:D:145:ARG:HD3	1:D:148:GLU:OE1	2.21	0.41
1:F:47:ASN:HB2	2:F:202:SO4:O4	2.19	0.41
1:F:90:LEU:HD13	1:F:94:THR:HG21	2.02	0.41
1:F:109:ASP:C	1:F:109:ASP:OD1	2.59	0.41
1:C:44:ILE:HD13	1:C:44:ILE:N	2.37	0.41
1:D:20:LYS:HA	1:D:24:LEU:HB2	2.02	0.41
1:A:8:GLU:HA	1:A:114:LEU:O	2.22	0.40
1:D:129:LYS:H	1:D:132:GLN:NE2	2.19	0.40
1:E:59:PRO:CD	1:E:62:PHE:CD2	2.97	0.40
1:A:54:LYS:HB2	1:A:54:LYS:HE3	1.65	0.40
1:D:4:ASN:HB2	1:D:119:LYS:HD3	2.04	0.40
1:E:58:PHE:HB3	1:E:59:PRO:HD2	2.02	0.40

All (3) 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)
2:E:201:SO4:O3	2:E:201:SO4:O3[2_655]	1.20	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:201:SO4:S	2:E:201:SO4:O3[2_655]	2.01	0.19
3:B:327:HOH:O	3:F:336:HOH:O[7_544]	2.18	0.02

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	158/159 (99%)	149 (94%)	9 (6%)	0	100	100
1	B	158/159 (99%)	151 (96%)	7 (4%)	0	100	100
1	C	159/159 (100%)	151 (95%)	8 (5%)	0	100	100
1	D	158/159 (99%)	149 (94%)	8 (5%)	1 (1%)	27	46
1	E	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	27	46
1	F	158/159 (99%)	153 (97%)	5 (3%)	0	100	100
All	All	948/954 (99%)	905 (96%)	41 (4%)	2 (0%)	49	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	GLY
1	E	60	GLU

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	136/135 (101%)	127 (93%)	9 (7%)	18	34
1	B	136/135 (101%)	128 (94%)	8 (6%)	21	40
1	C	137/135 (102%)	124 (90%)	13 (10%)	9	18
1	D	136/135 (101%)	124 (91%)	12 (9%)	11	21
1	E	134/135 (99%)	122 (91%)	12 (9%)	10	20
1	F	136/135 (101%)	121 (89%)	15 (11%)	7	13
All	All	815/810 (101%)	746 (92%)	69 (8%)	12	22

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	38	ILE
1	A	47	ASN
1	A	69	ILE
1	A	90	LEU
1	A	94	THR
1	A	105	VAL
1	A	136	SER
1	A	137	LYS
1	B	12	VAL
1	B	33	VAL
1	B	69	ILE
1	B	94	THR
1	B	95	LEU
1	B	109	ASP
1	B	119	LYS
1	B	149	SER
1	C	2	VAL
1	C	7	THR
1	C	9	THR
1	C	47	ASN
1	C	57	SER
1	C	77	THR
1	C	94	THR
1	C	114	LEU
1	C	116	ILE
1	C	137	LYS
1	C	139	MET
1	C	145	ARG
1	C	149	SER

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Mol	Chain	Res	Type
1	E	12	VAL
1	E	29	LEU
1	E	47	ASN
1	E	65	LYS
1	E	94	THR
1	E	95	LEU
1	E	99	SER
1	E	105	VAL
1	E	109	ASP
1	E	119	LYS
1	E	123	LYS
1	E	142	THR
1	F	2	VAL
1	F	8	GLU
1	F	9	THR
1	F	20	LYS
1	F	42	GLU
1	F	93	ASP
1	F	94	THR
1	F	96	GLU
1	F	99	SER
1	F	116	ILE
1	F	125	ASP
1	F	136	SER
1	F	137	LYS
1	F	142	THR
1	F	149	SER
1	D	9	THR
1	D	24	LEU
1	D	60	GLU
1	D	93	ASP
1	D	95	LEU
1	D	105	VAL
1	D	125	ASP
1	D	131	GLU
1	D	132	GLN
1	D	139	MET
1	D	148	GLU
1	D	156	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	28	ASN
1	A	82	ASN
1	A	118	ASN
1	B	118	ASN
1	B	121	HIS
1	B	132	GLN
1	C	4	ASN
1	C	118	ASN
1	C	121	HIS
1	C	132	GLN
1	E	82	ASN
1	E	100	ASN
1	E	159	ASN
1	F	118	ASN
1	F	121	HIS
1	F	154	HIS
1	D	47	ASN
1	D	100	ASN
1	D	118	ASN
1	D	126	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 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	201	-	4,4,4	0.57	0	6,6,6	0.94	0
2	SO4	A	202	-	4,4,4	0.51	0	6,6,6	0.54	0
2	SO4	A	203	-	4,4,4	0.49	0	6,6,6	0.18	0
2	SO4	B	201	-	4,4,4	0.50	0	6,6,6	0.26	0
2	SO4	B	202	-	4,4,4	0.64	0	6,6,6	0.97	0
2	SO4	B	203	-	4,4,4	0.47	0	6,6,6	0.24	0
2	SO4	B	204	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	C	201	-	4,4,4	0.49	0	6,6,6	0.74	0
2	SO4	E	201	-	4,4,4	0.51	0	6,6,6	0.38	0
2	SO4	F	201	-	4,4,4	0.33	0	6,6,6	0.35	0
2	SO4	F	202	-	4,4,4	0.47	0	6,6,6	0.31	0
2	SO4	F	203	-	4,4,4	0.49	0	6,6,6	0.32	0
2	SO4	F	204	-	4,4,4	0.55	0	6,6,6	0.25	0
2	SO4	F	205	-	4,4,4	0.44	0	6,6,6	0.79	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	201	-	-	0/0/0/0	0/0/0/0
2	SO4	A	202	-	-	0/0/0/0	0/0/0/0
2	SO4	A	203	-	-	0/0/0/0	0/0/0/0
2	SO4	B	201	-	-	0/0/0/0	0/0/0/0
2	SO4	B	202	-	-	0/0/0/0	0/0/0/0
2	SO4	B	203	-	-	0/0/0/0	0/0/0/0
2	SO4	B	204	-	-	0/0/0/0	0/0/0/0
2	SO4	C	201	-	-	0/0/0/0	0/0/0/0
2	SO4	E	201	-	-	0/0/0/0	0/0/0/0
2	SO4	F	201	-	-	0/0/0/0	0/0/0/0
2	SO4	F	202	-	-	0/0/0/0	0/0/0/0
2	SO4	F	203	-	-	0/0/0/0	0/0/0/0
2	SO4	F	204	-	-	0/0/0/0	0/0/0/0
2	SO4	F	205	-	-	0/0/0/0	0/0/0/0

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.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	202	SO4	2	0
2	C	201	SO4	1	0
2	E	201	SO4	0	2
2	F	202	SO4	1	0
2	F	205	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	69:ILE	C	70:ARG	N	1.19

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	159/159 (100%)	-0.17	2 (1%) 77 78	15, 25, 45, 55	0
1	B	159/159 (100%)	-0.20	2 (1%) 77 78	14, 23, 42, 59	0
1	C	159/159 (100%)	0.13	5 (3%) 49 52	14, 29, 48, 65	0
1	D	159/159 (100%)	0.20	8 (5%) 29 31	16, 31, 51, 82	0
1	E	159/159 (100%)	-0.03	6 (3%) 40 43	18, 28, 50, 92	0
1	F	159/159 (100%)	-0.09	5 (3%) 49 52	17, 27, 52, 64	0
All	All	954/954 (100%)	-0.03	28 (2%) 51 55	14, 27, 47, 92	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	61	GLY	5.4
1	D	159	ASN	4.4
1	F	159	ASN	3.8
1	D	77	THR	3.7
1	D	61	GLY	3.7
1	B	60	GLU	3.6
1	C	5[A]	TYR	3.4
1	D	62	PHE	3.4
1	E	60	GLU	3.3
1	F	64	PHE	3.2
1	D	60	GLU	3.1
1	F	62	PHE	2.9
1	E	63	PRO	2.9
1	E	62	PHE	2.7
1	E	64	PHE	2.7
1	D	78	ASN	2.5
1	E	157	ALA	2.5
1	F	156	ASP	2.5
1	A	64	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	13	ILE	2.4
1	C	77	THR	2.3
1	F	125	ASP	2.3
1	C	60	GLU	2.3
1	A	62	PHE	2.2
1	C	61	GLY	2.2
1	B	64	PHE	2.1
1	D	16	ALA	2.1
1	D	47	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. 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	B-factors(Å ²)	Q<0.9
2	SO4	F	205	5/5	0.78	0.31	63,64,83,97	0
2	SO4	B	202	5/5	0.79	0.30	61,69,84,90	0
2	SO4	C	201	5/5	0.81	0.36	71,85,88,91	0
2	SO4	F	203	5/5	0.85	0.33	82,83,87,92	0
2	SO4	A	202	5/5	0.89	0.31	79,85,88,90	0
2	SO4	F	204	5/5	0.89	0.24	66,73,81,85	0
2	SO4	B	203	5/5	0.90	0.19	76,78,90,94	0
2	SO4	A	203	5/5	0.90	0.20	93,94,105,105	0
2	SO4	A	201	5/5	0.93	0.18	47,48,48,54	0
2	SO4	F	202	5/5	0.95	0.20	64,66,73,76	0
2	SO4	B	204	5/5	0.96	0.13	49,50,54,57	0
2	SO4	B	201	5/5	0.97	0.13	52,53,53,54	0
2	SO4	E	201	5/5	0.97	0.18	34,37,139,143	2
2	SO4	F	201	5/5	0.98	0.11	41,44,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.