Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2021 – 04:16 PM EDT

PDB ID	:	3ENM
Title	:	The structure of the MAP2K MEK6 reveals an autoinhibitory dimer
Authors	:	Min, X.; Akella, R.; He, H.; Humphreys, J.M.; Tsutakawa, S.; Lee, S.-J.; Tainer, J.A.; Cobb, M.H.; Goldsmith, E.J.
Deposited on	:	2008-09-25
Resolution	:	2.35 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 following versions of software and data (see references (i)) were used in the production of this report:

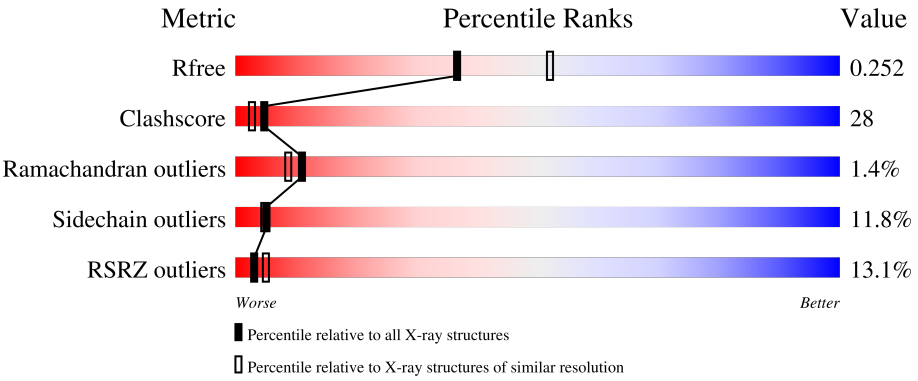
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	9% 58% 24% 6% • 12%
1	B	316	12% 51% 28% 7% • 14%
1	C	316	9% 52% 27% 8% • 13%
1	D	316	14% 59% 25% • • 11%

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	4	-	-	X	-
3	GOL	A	1	-	-	X	X
4	EDO	B	1	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9174 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 Dual specificity mitogen-activated protein kinase kinase 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	Se	0	0	0
			2223	1429	368	411	4	11			
1	B	271	Total	C	N	O	S	Se	20	1	0
			2163	1388	360	400	4	11			
1	C	275	Total	C	N	O	S	Se	7	0	0
			2185	1403	363	404	4	11			
1	D	282	Total	C	N	O	S	Se	0	0	0
			2248	1443	372	417	4	12			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MSE	-	expression tag	UNP P52564
A	19	SER	-	expression tag	UNP P52564
A	20	TYR	-	expression tag	UNP P52564
A	21	TYR	-	expression tag	UNP P52564
A	22	HIS	-	expression tag	UNP P52564
A	23	HIS	-	expression tag	UNP P52564
A	24	HIS	-	expression tag	UNP P52564
A	25	HIS	-	expression tag	UNP P52564
A	26	HIS	-	expression tag	UNP P52564
A	27	HIS	-	expression tag	UNP P52564
A	28	ASP	-	expression tag	UNP P52564
A	29	TYR	-	expression tag	UNP P52564
A	30	ASP	-	expression tag	UNP P52564
A	31	ILE	-	expression tag	UNP P52564
A	32	PRO	-	expression tag	UNP P52564
A	33	THR	-	expression tag	UNP P52564
A	34	THR	-	expression tag	UNP P52564
A	35	GLU	-	expression tag	UNP P52564
A	36	ASN	-	expression tag	UNP P52564
A	37	LEU	-	expression tag	UNP P52564
A	38	TYR	-	expression tag	UNP P52564

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Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PHE	-	expression tag	UNP P52564
A	40	GLN	-	expression tag	UNP P52564
A	41	GLY	-	expression tag	UNP P52564
A	42	ALA	-	expression tag	UNP P52564
A	43	MSE	-	expression tag	UNP P52564
A	44	GLU	-	expression tag	UNP P52564
A	207	ASP	SER	engineered mutation	UNP P52564
A	211	ASP	THR	engineered mutation	UNP P52564
A	333	ALA	-	expression tag	UNP P52564
B	18	MSE	-	expression tag	UNP P52564
B	19	SER	-	expression tag	UNP P52564
B	20	TYR	-	expression tag	UNP P52564
B	21	TYR	-	expression tag	UNP P52564
B	22	HIS	-	expression tag	UNP P52564
B	23	HIS	-	expression tag	UNP P52564
B	24	HIS	-	expression tag	UNP P52564
B	25	HIS	-	expression tag	UNP P52564
B	26	HIS	-	expression tag	UNP P52564
B	27	HIS	-	expression tag	UNP P52564
B	28	ASP	-	expression tag	UNP P52564
B	29	TYR	-	expression tag	UNP P52564
B	30	ASP	-	expression tag	UNP P52564
B	31	ILE	-	expression tag	UNP P52564
B	32	PRO	-	expression tag	UNP P52564
B	33	THR	-	expression tag	UNP P52564
B	34	THR	-	expression tag	UNP P52564
B	35	GLU	-	expression tag	UNP P52564
B	36	ASN	-	expression tag	UNP P52564
B	37	LEU	-	expression tag	UNP P52564
B	38	TYR	-	expression tag	UNP P52564
B	39	PHE	-	expression tag	UNP P52564
B	40	GLN	-	expression tag	UNP P52564
B	41	GLY	-	expression tag	UNP P52564
B	42	ALA	-	expression tag	UNP P52564
B	43	MSE	-	expression tag	UNP P52564
B	44	GLU	-	expression tag	UNP P52564
B	207	ASP	SER	engineered mutation	UNP P52564
B	211	ASP	THR	engineered mutation	UNP P52564
B	333	ALA	-	expression tag	UNP P52564
C	18	MSE	-	expression tag	UNP P52564
C	19	SER	-	expression tag	UNP P52564
C	20	TYR	-	expression tag	UNP P52564

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	TYR	-	expression tag	UNP P52564
C	22	HIS	-	expression tag	UNP P52564
C	23	HIS	-	expression tag	UNP P52564
C	24	HIS	-	expression tag	UNP P52564
C	25	HIS	-	expression tag	UNP P52564
C	26	HIS	-	expression tag	UNP P52564
C	27	HIS	-	expression tag	UNP P52564
C	28	ASP	-	expression tag	UNP P52564
C	29	TYR	-	expression tag	UNP P52564
C	30	ASP	-	expression tag	UNP P52564
C	31	ILE	-	expression tag	UNP P52564
C	32	PRO	-	expression tag	UNP P52564
C	33	THR	-	expression tag	UNP P52564
C	34	THR	-	expression tag	UNP P52564
C	35	GLU	-	expression tag	UNP P52564
C	36	ASN	-	expression tag	UNP P52564
C	37	LEU	-	expression tag	UNP P52564
C	38	TYR	-	expression tag	UNP P52564
C	39	PHE	-	expression tag	UNP P52564
C	40	GLN	-	expression tag	UNP P52564
C	41	GLY	-	expression tag	UNP P52564
C	42	ALA	-	expression tag	UNP P52564
C	43	MSE	-	expression tag	UNP P52564
C	44	GLU	-	expression tag	UNP P52564
C	207	ASP	SER	engineered mutation	UNP P52564
C	211	ASP	THR	engineered mutation	UNP P52564
C	333	ALA	-	expression tag	UNP P52564
D	18	MSE	-	expression tag	UNP P52564
D	19	SER	-	expression tag	UNP P52564
D	20	TYR	-	expression tag	UNP P52564
D	21	TYR	-	expression tag	UNP P52564
D	22	HIS	-	expression tag	UNP P52564
D	23	HIS	-	expression tag	UNP P52564
D	24	HIS	-	expression tag	UNP P52564
D	25	HIS	-	expression tag	UNP P52564
D	26	HIS	-	expression tag	UNP P52564
D	27	HIS	-	expression tag	UNP P52564
D	28	ASP	-	expression tag	UNP P52564
D	29	TYR	-	expression tag	UNP P52564
D	30	ASP	-	expression tag	UNP P52564
D	31	ILE	-	expression tag	UNP P52564
D	32	PRO	-	expression tag	UNP P52564

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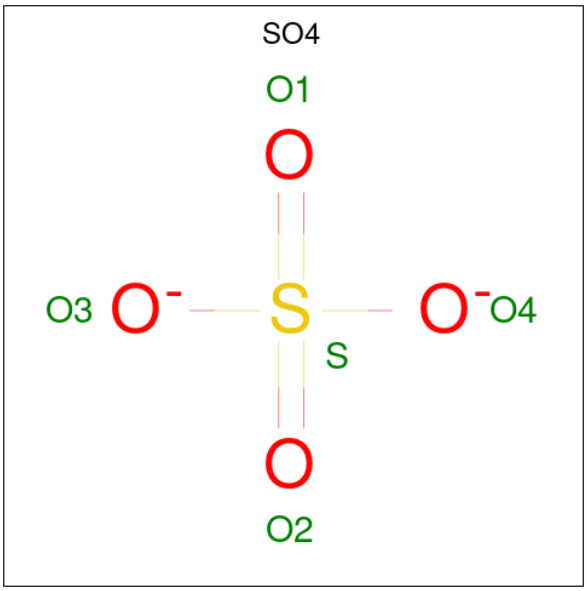
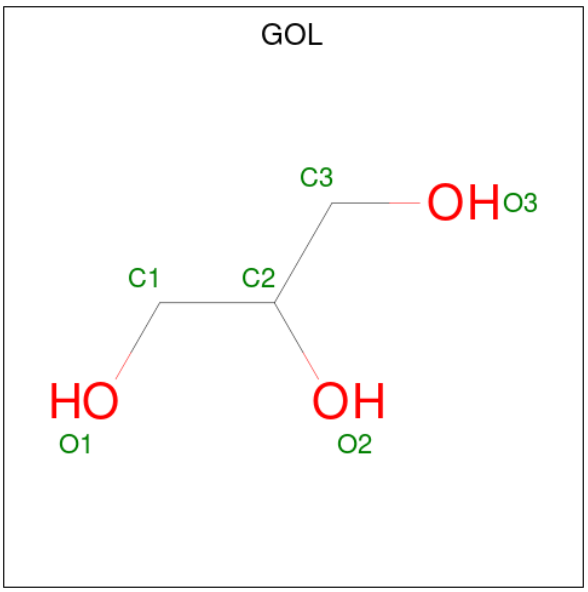
Chain	Residue	Modelled	Actual	Comment	Reference
D	33	THR	-	expression tag	UNP P52564
D	34	THR	-	expression tag	UNP P52564
D	35	GLU	-	expression tag	UNP P52564
D	36	ASN	-	expression tag	UNP P52564
D	37	LEU	-	expression tag	UNP P52564
D	38	TYR	-	expression tag	UNP P52564
D	39	PHE	-	expression tag	UNP P52564
D	40	GLN	-	expression tag	UNP P52564
D	41	GLY	-	expression tag	UNP P52564
D	42	ALA	-	expression tag	UNP P52564
D	43	MSE	-	expression tag	UNP P52564
D	44	GLU	-	expression tag	UNP P52564
D	207	ASP	SER	engineered mutation	UNP P52564
D	211	ASP	THR	engineered mutation	UNP P52564
D	333	ALA	-	expression tag	UNP P52564

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



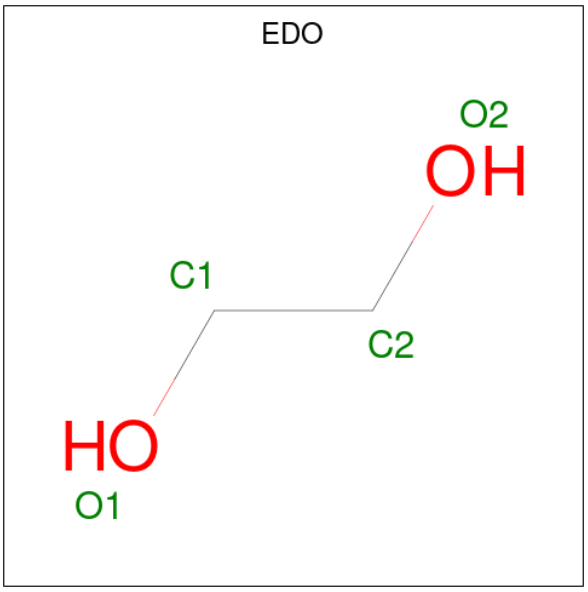
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

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



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

- Molecule 5 is water.

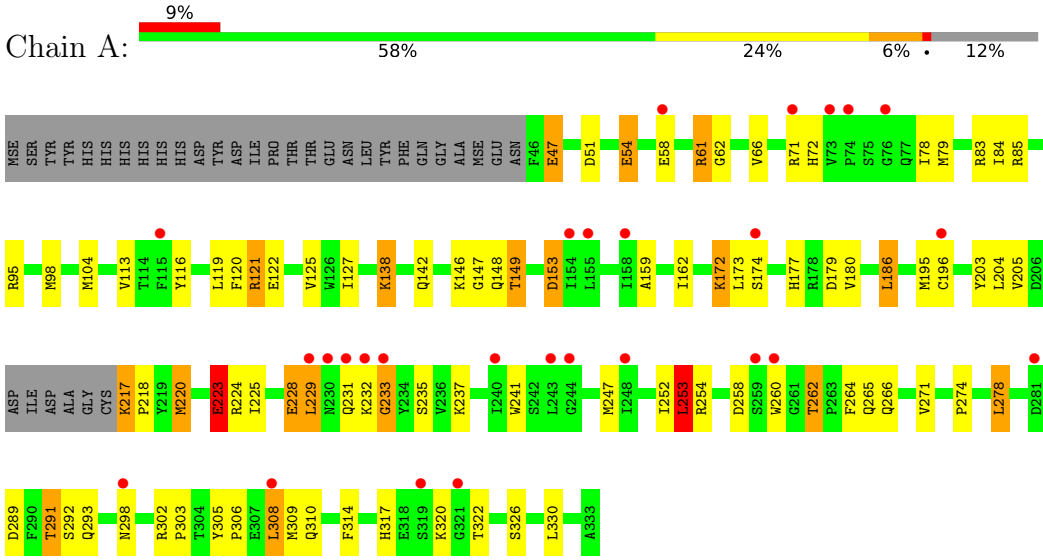
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	93	Total O 93 93	0	0
5	B	74	Total O 74 74	0	0
5	C	78	Total O 78 78	0	0
5	D	80	Total O 80 80	0	0

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.

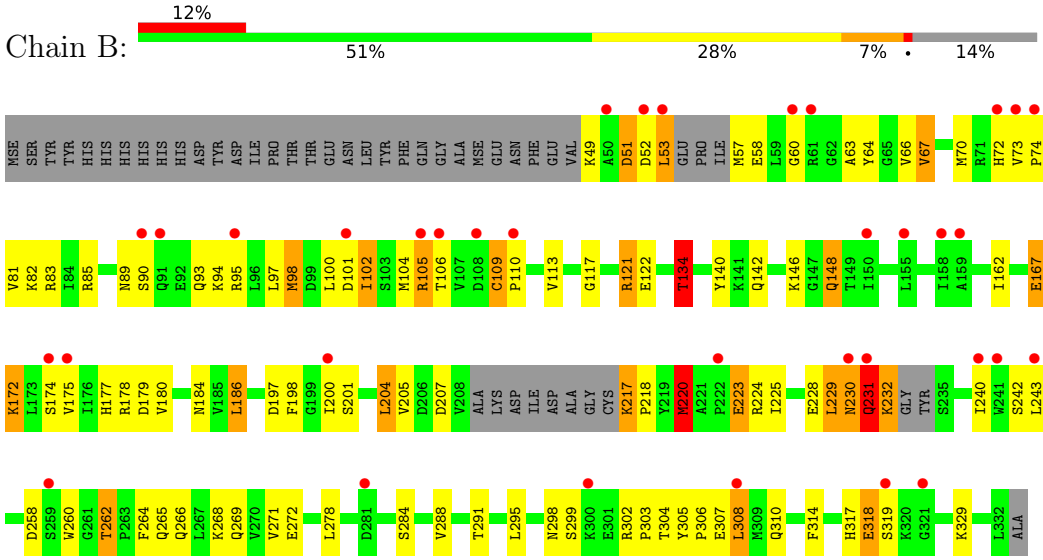
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6

Chain A:



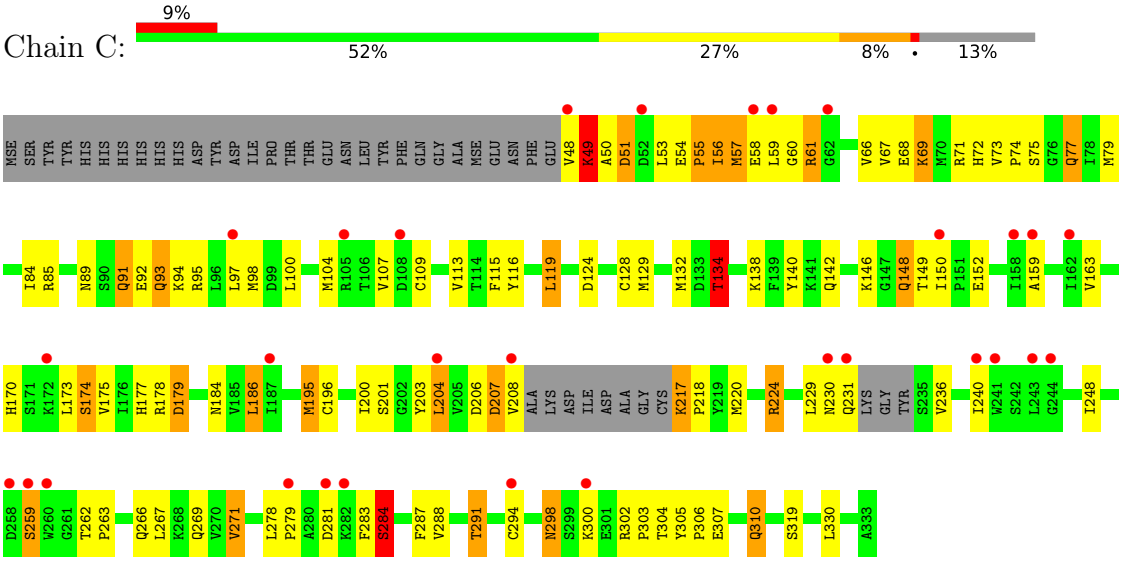
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6

Chain B:



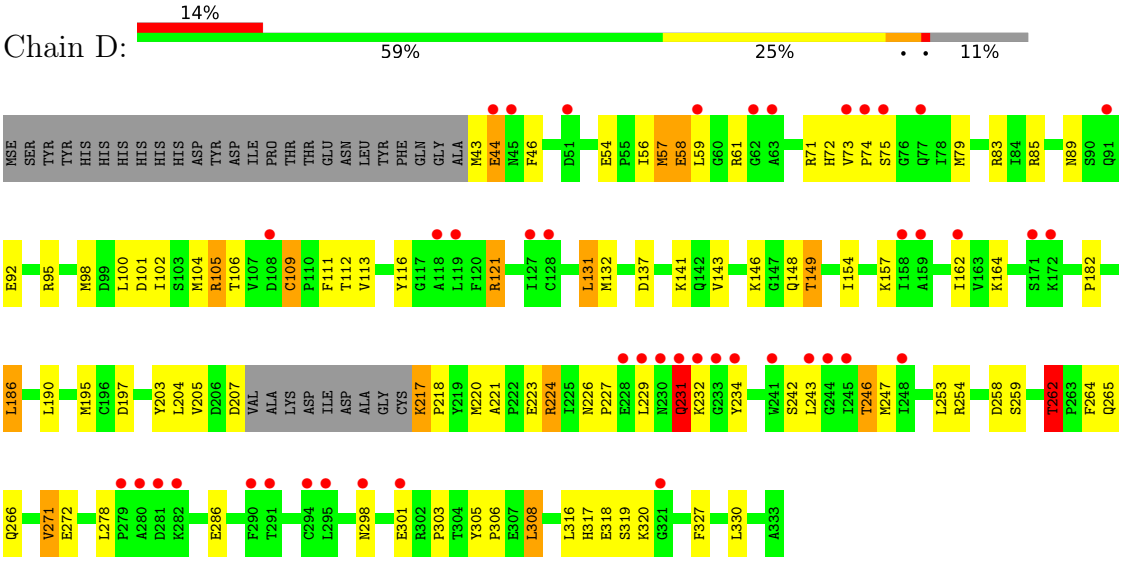
• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6

Chain C:



• Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.66Å 122.66Å 195.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.35 19.97 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.97-2.35) 99.3 (19.97-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.212 , 0.269 0.207 , 0.252	Depositor DCC
R_{free} test set	3582 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 69.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9174	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, EDO, GOL

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	0.88	2/2260 (0.1%)	0.91	2/3035 (0.1%)
1	B	0.86	0/2199	0.92	3/2950 (0.1%)
1	C	0.83	0/2219	0.89	1/2980 (0.0%)
1	D	0.81	0/2285	0.89	1/3068 (0.0%)
All	All	0.85	2/8963 (0.0%)	0.90	7/12033 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	GLU	CB-CG	5.51	1.62	1.52
1	A	223	GLU	CB-CG	-5.40	1.41	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	224	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	134	THR	CB-CA-C	-5.63	96.38	111.60
1	A	253	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	B	220	MSE	CG-SE-CE	-5.34	87.15	98.90
1	C	134	THR	CB-CA-C	-5.30	97.28	111.60
1	D	262	THR	N-CA-CB	-5.04	100.72	110.30
1	B	260	TRP	CB-CG-CD1	5.03	133.53	127.00

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	2223	0	2248	120	0
1	B	2163	0	2194	128	0
1	C	2185	0	2215	157	0
1	D	2248	0	2269	109	0
2	A	5	0	0	1	0
2	B	5	0	0	5	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	6	0	8	7	0
4	B	4	0	6	7	0
5	A	93	0	0	8	0
5	B	74	0	0	12	0
5	C	78	0	0	9	0
5	D	80	0	0	4	0
All	All	9174	0	8940	494	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 28.

All (494) 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:56:ILE:CG2	1:C:57:MSE:N	1.70	1.41
1:A:119:LEU:HD21	1:C:208:VAL:CG1	1.46	1.41
1:A:119:LEU:CD2	1:C:208:VAL:HG11	1.55	1.33
1:C:177:HIS:CD2	1:C:179:ASP:H	1.50	1.30
1:D:43:MSE:O	1:D:44:GLU:HG3	1.43	1.18
1:C:56:ILE:HG22	1:C:57:MSE:N	1.21	1.17
1:A:159:ALA:HA	1:A:247:MSE:CE	1.77	1.15
1:C:177:HIS:HD2	1:C:179:ASP:N	1.45	1.13
1:D:162:ILE:HD12	1:D:247:MSE:HE1	1.31	1.13
1:B:217:LYS:HB3	1:B:218:PRO:CD	1.80	1.11
1:A:220:MSE:HE3	1:A:225:ILE:HD11	1.30	1.10
1:A:274:PRO:HA	3:A:1:GOL:C3	1.82	1.09
1:B:93:GLN:O	1:B:97:LEU:HG	1.51	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ILE:HG23	1:C:57:MSE:N	1.68	1.08
1:C:89:ASN:OD1	1:C:91:GLN:HG3	1.53	1.08
1:C:217:LYS:HD2	5:C:467:HOH:O	1.52	1.08
1:A:159:ALA:HA	1:A:247:MSE:HE3	1.11	1.08
1:D:95:ARG:NH2	1:D:98:MSE:HE2	1.67	1.08
1:A:253:LEU:N	1:A:253:LEU:HD22	1.62	1.06
1:D:231:GLN:HG2	1:D:232:LYS:N	1.68	1.06
1:B:217:LYS:HB3	1:B:218:PRO:HD3	1.32	1.06
1:D:231:GLN:CD	1:D:232:LYS:H	1.58	1.05
1:B:262:THR:HG22	1:B:265:GLN:H	1.18	1.05
1:A:274:PRO:HB3	3:A:1:GOL:H32	1.37	1.05
1:C:55:PRO:HD3	1:C:71:ARG:O	1.55	1.05
1:D:231:GLN:CG	1:D:232:LYS:H	1.68	1.04
1:D:231:GLN:CG	1:D:232:LYS:N	2.19	1.04
1:A:274:PRO:HA	3:A:1:GOL:H31	1.36	1.04
1:B:49:LYS:HB3	1:B:117:GLY:HA3	1.38	1.04
1:B:83:ARG:H	4:B:1:EDO:H22	1.23	1.04
1:C:230:ASN:O	1:C:231:GLN:HG3	1.57	1.03
1:A:229:LEU:HD22	1:A:229:LEU:O	1.59	1.01
1:B:248:ILE:HD11	1:B:291:THR:HG21	1.38	1.01
1:B:319:SER:HB3	5:B:386:HOH:O	1.61	1.00
1:A:121:ARG:HG3	1:C:208:VAL:HG13	1.42	1.00
1:C:152:GLU:OE2	1:C:284:SER:HB2	1.61	1.00
1:C:259:SER:HB3	1:C:266:GLN:HG2	1.45	0.99
1:C:55:PRO:HG3	1:C:71:ARG:HB3	1.44	0.99
1:A:274:PRO:CB	3:A:1:GOL:H32	1.93	0.98
1:A:159:ALA:CA	1:A:247:MSE:HE3	1.94	0.98
1:C:91:GLN:HE21	1:C:92:GLU:N	1.61	0.97
1:A:262:THR:HG22	1:A:265:GLN:H	1.29	0.97
1:C:55:PRO:CG	1:C:71:ARG:HB3	1.95	0.97
1:A:218:PRO:HB3	1:A:220:MSE:HE1	1.45	0.96
1:C:55:PRO:O	1:C:56:ILE:HG13	1.65	0.96
1:A:326:SER:O	1:A:330:LEU:HD23	1.66	0.96
1:B:248:ILE:HD11	1:B:291:THR:CG2	1.97	0.95
1:B:100:LEU:HG	1:B:104:MSE:HE2	1.45	0.94
1:A:177:HIS:HD2	1:A:179:ASP:H	1.01	0.93
1:C:48:VAL:HG12	1:C:49:LYS:HG2	1.49	0.92
1:A:274:PRO:CA	3:A:1:GOL:H32	2.01	0.89
1:B:52:ASP:OD2	1:B:72:HIS:HE1	1.55	0.88
1:A:229:LEU:HD22	1:A:229:LEU:C	1.88	0.88
1:A:218:PRO:CB	1:A:220:MSE:HE1	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:MSE:HE2	1:D:58:GLU:O	1.72	0.88
1:C:291:THR:HG22	5:C:441:HOH:O	1.73	0.87
1:D:262:THR:HG22	1:D:265:GLN:H	1.39	0.87
1:B:231:GLN:HG2	1:B:232:LYS:N	1.88	0.87
1:D:217:LYS:HG2	1:D:266:GLN:OE1	1.75	0.87
1:B:205:VAL:HB	4:B:1:EDO:H12	1.54	0.86
1:D:182:PRO:HD3	1:D:246:THR:HB	1.57	0.86
1:C:48:VAL:HG13	1:C:49:LYS:HD3	1.54	0.86
1:D:43:MSE:O	1:D:44:GLU:CG	2.23	0.86
1:C:55:PRO:O	1:C:56:ILE:CG1	2.24	0.85
1:C:91:GLN:HE21	1:C:92:GLU:CA	1.88	0.85
1:C:67:VAL:O	1:C:68:GLU:HB2	1.74	0.85
1:C:50:ALA:O	1:C:51:ASP:CB	2.24	0.84
1:B:52:ASP:O	1:B:53:LEU:HB2	1.75	0.84
1:C:291:THR:CG2	5:C:441:HOH:O	2.22	0.84
1:D:243:LEU:HD11	1:D:247:MSE:HE3	1.59	0.84
1:A:274:PRO:HA	3:A:1:GOL:H32	1.59	0.83
1:B:94:LYS:HG2	1:B:98:MSE:HE3	1.58	0.83
1:C:104:MSE:HG2	1:C:115:PHE:O	1.78	0.83
1:D:95:ARG:NH2	1:D:98:MSE:CE	2.41	0.83
1:B:52:ASP:OD2	1:B:72:HIS:CE1	2.32	0.83
1:C:206:ASP:O	1:C:207:ASP:CB	2.27	0.83
1:D:95:ARG:HH21	1:D:98:MSE:HE2	1.41	0.82
1:A:253:LEU:N	1:A:253:LEU:CD2	2.42	0.82
1:B:134:THR:HG23	5:B:361:HOH:O	1.80	0.82
1:A:274:PRO:CA	3:A:1:GOL:C3	2.57	0.81
1:B:217:LYS:HD3	1:B:266:GLN:OE1	1.79	0.81
1:A:232:LYS:NZ	1:A:232:LYS:HB3	1.95	0.81
1:A:142:GLN:NE2	1:A:146:LYS:HE3	1.97	0.80
1:A:162:ILE:HD12	1:A:247:MSE:HE1	1.63	0.80
1:B:83:ARG:H	4:B:1:EDO:C2	1.94	0.80
1:A:220:MSE:HE3	1:A:225:ILE:CD1	2.11	0.80
1:A:225:ILE:O	1:B:262:THR:HG21	1.81	0.80
1:C:152:GLU:OE2	1:C:284:SER:CB	2.30	0.80
1:C:177:HIS:CD2	1:C:179:ASP:N	2.29	0.80
1:D:113:VAL:HG11	1:D:186:LEU:HD22	1.64	0.80
1:B:200:ILE:HG13	1:B:204:LEU:HD22	1.63	0.79
1:A:153:ASP:OD1	1:A:320:LYS:HE2	1.83	0.79
1:C:177:HIS:O	1:C:178:ARG:HG2	1.83	0.78
1:A:252:ILE:C	1:A:253:LEU:HD22	2.03	0.78
1:A:262:THR:HG21	1:B:225:ILE:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HD12	1:A:247:MSE:CE	2.14	0.78
1:C:217:LYS:HB2	1:C:217:LYS:NZ	1.99	0.77
1:A:113:VAL:HG21	1:A:186:LEU:HD22	1.66	0.77
1:D:231:GLN:OE1	1:D:232:LYS:N	2.16	0.77
1:A:220:MSE:CE	1:A:225:ILE:HD11	2.13	0.77
1:C:217:LYS:HB2	1:C:217:LYS:HZ2	1.50	0.76
1:D:303:PRO:HG2	1:D:308:LEU:HD13	1.68	0.76
1:D:243:LEU:CD1	1:D:247:MSE:HE3	2.15	0.76
1:C:50:ALA:O	1:C:51:ASP:HB3	1.83	0.75
1:B:93:GLN:HB3	2:B:4:SO4:S	2.26	0.75
1:B:248:ILE:CD1	1:B:291:THR:HG21	2.15	0.75
1:D:43:MSE:HG3	1:D:46:PHE:CD2	2.21	0.75
1:D:243:LEU:CD1	1:D:247:MSE:CE	2.64	0.75
1:C:206:ASP:O	1:C:207:ASP:HB2	1.85	0.75
1:C:259:SER:CB	1:C:266:GLN:HG2	2.17	0.75
1:C:294:CYS:O	1:C:302:ARG:HD3	1.87	0.74
1:A:232:LYS:HB3	1:A:232:LYS:HZ2	1.49	0.74
1:C:56:ILE:HG22	1:C:57:MSE:CA	2.17	0.74
1:D:131:LEU:CD1	1:D:131:LEU:C	2.55	0.74
1:A:177:HIS:CD2	1:A:179:ASP:H	1.94	0.73
1:C:200:ILE:HG13	1:C:204:LEU:HD22	1.68	0.73
1:A:159:ALA:CA	1:A:247:MSE:CE	2.62	0.73
1:D:262:THR:H	1:D:265:GLN:HE21	1.37	0.73
1:B:109:CYS:SG	1:B:110:PRO:HD2	2.29	0.73
1:A:119:LEU:HD21	1:C:208:VAL:HG11	0.76	0.73
1:A:119:LEU:HD21	1:C:208:VAL:HG12	1.63	0.73
1:A:320:LYS:HE3	5:A:383:HOH:O	1.87	0.72
1:D:162:ILE:CD1	1:D:247:MSE:HE1	2.17	0.72
1:A:84:ILE:HD11	1:A:127:ILE:HD11	1.72	0.72
1:C:55:PRO:CD	1:C:71:ARG:O	2.37	0.71
1:A:217:LYS:HE3	1:A:266:GLN:NE2	2.05	0.71
1:C:230:ASN:HA	5:C:419:HOH:O	1.89	0.71
1:D:131:LEU:HD13	1:D:132:MSE:N	2.06	0.71
1:C:50:ALA:HB1	1:C:53:LEU:HG	1.73	0.71
1:A:177:HIS:HD2	1:A:179:ASP:N	1.84	0.71
1:C:50:ALA:HB2	1:C:53:LEU:HD12	1.71	0.71
1:D:43:MSE:HB3	1:D:46:PHE:HB3	1.71	0.71
1:B:72:HIS:HD2	1:B:75:SER:OG	1.74	0.70
1:B:83:ARG:N	4:B:1:EDO:H22	2.01	0.70
1:B:284:SER:O	1:B:288:VAL:HG23	1.91	0.70
1:C:55:PRO:HG2	1:C:71:ARG:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASP:OD2	1:B:74:PRO:HG2	1.91	0.70
1:B:298:ASN:OD1	1:B:298:ASN:C	2.28	0.70
1:D:79:MSE:HE2	1:D:116:TYR:CD2	2.26	0.70
1:B:205:VAL:HB	4:B:1:EDO:C1	2.21	0.70
1:C:284:SER:O	1:C:288:VAL:HG23	1.91	0.70
1:A:89:ASN:HB2	2:A:2:SO4:O3	1.92	0.69
1:A:54:GLU:OE1	1:A:71:ARG:NH1	2.25	0.69
1:C:55:PRO:HG3	1:C:71:ARG:CB	2.21	0.69
1:B:72:HIS:HD2	1:B:75:SER:CB	2.05	0.69
1:C:77:GLN:NE2	1:C:116:TYR:OH	2.25	0.69
1:A:217:LYS:HG3	1:A:218:PRO:HD3	1.75	0.69
1:A:83:ARG:HH22	1:C:124:ASP:CG	1.95	0.69
1:D:121:ARG:HH11	1:D:121:ARG:HG3	1.57	0.68
1:B:304:THR:HG23	1:B:307:GLU:OE1	1.92	0.68
1:C:113:VAL:HG21	1:C:186:LEU:HD22	1.74	0.68
1:A:252:ILE:C	1:A:253:LEU:CD2	2.62	0.68
1:B:94:LYS:O	1:B:97:LEU:HB2	1.94	0.68
1:C:50:ALA:CB	1:C:53:LEU:HD12	2.24	0.68
1:A:142:GLN:NE2	1:A:146:LYS:CE	2.56	0.67
1:A:217:LYS:HE3	1:A:266:GLN:HE22	1.60	0.67
1:C:53:LEU:HD22	1:D:190:LEU:HD11	1.77	0.67
1:D:243:LEU:HD12	1:D:247:MSE:HE2	1.77	0.67
1:D:57:MSE:CE	1:D:58:GLU:O	2.43	0.67
1:A:121:ARG:HG3	1:C:208:VAL:CG1	2.21	0.67
1:B:73:VAL:N	1:B:74:PRO:CD	2.58	0.66
1:C:56:ILE:CG2	1:C:57:MSE:O	2.43	0.66
1:C:224:ARG:NH2	1:C:231:GLN:O	2.28	0.66
1:C:48:VAL:CG1	1:C:49:LYS:HG2	2.24	0.66
1:C:89:ASN:HB2	2:C:3:SO4:O1	1.96	0.66
1:C:298:ASN:C	1:C:298:ASN:HD22	2.00	0.66
1:B:93:GLN:O	1:B:97:LEU:CG	2.38	0.65
1:A:284:SER:O	1:A:288:VAL:HG23	1.96	0.65
1:C:267:LEU:O	1:C:271:VAL:HG12	1.96	0.65
1:B:262:THR:HG22	1:B:265:GLN:N	2.03	0.65
1:D:101:ASP:OD1	1:D:105:ARG:NH2	2.20	0.65
1:A:47:GLU:OE2	1:A:120:PHE:HD1	1.81	0.64
1:A:207:ASP:HB3	1:C:66:VAL:HG22	1.80	0.64
1:C:50:ALA:HB1	1:C:53:LEU:CG	2.27	0.64
1:C:217:LYS:HB3	1:C:218:PRO:HD3	1.79	0.64
1:C:53:LEU:HD22	1:D:190:LEU:CD1	2.28	0.63
1:A:278:LEU:HB2	1:A:291:THR:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:HD3	5:A:398:HOH:O	1.98	0.63
1:A:172:LYS:C	1:A:173:LEU:HD23	2.19	0.63
1:A:232:LYS:O	1:A:233:GLY:O	2.17	0.63
1:D:95:ARG:HH22	1:D:98:MSE:HE2	1.59	0.63
1:D:217:LYS:HB3	1:D:218:PRO:CD	2.29	0.62
1:C:59:LEU:HG	1:C:60:GLY:H	1.63	0.62
1:C:173:LEU:O	1:C:175:VAL:HG23	1.98	0.62
1:D:224:ARG:HD2	1:D:234:TYR:CE1	2.33	0.62
1:A:153:ASP:OD1	1:A:320:LYS:CE	2.48	0.62
1:B:197:ASP:OD2	1:B:198:PHE:HD2	1.83	0.62
1:A:138:LYS:HE3	5:A:397:HOH:O	2.00	0.62
1:B:314:PHE:CE2	1:B:318:GLU:HG3	2.35	0.62
1:A:262:THR:HG22	1:A:265:GLN:N	2.08	0.62
1:A:148:GLN:HG3	1:A:149:THR:H	1.65	0.61
1:B:73:VAL:N	1:B:74:PRO:HD2	2.15	0.61
1:D:131:LEU:C	1:D:131:LEU:HD13	2.21	0.61
1:C:48:VAL:O	1:C:49:LYS:O	2.19	0.61
1:D:242:SER:O	1:D:246:THR:HG23	1.99	0.61
1:A:83:ARG:NH2	1:C:124:ASP:OD1	2.34	0.61
1:C:159:ALA:O	1:C:163:VAL:HG23	2.01	0.61
1:A:262:THR:CG2	1:A:264:PHE:HB3	2.31	0.61
1:D:243:LEU:CD1	1:D:247:MSE:HE2	2.30	0.61
1:B:148:GLN:HG3	5:B:351:HOH:O	2.00	0.60
1:B:303:PRO:CG	1:B:308:LEU:HD13	2.31	0.60
1:D:72:HIS:HD2	1:D:75:SER:H	1.49	0.60
1:C:100:LEU:HG	1:C:104:MSE:HE2	1.83	0.60
1:C:170:HIS:O	1:C:174:SER:HA	2.01	0.60
1:B:93:GLN:HB3	2:B:4:SO4:O4	2.02	0.59
1:B:148:GLN:CG	5:B:351:HOH:O	2.50	0.59
1:A:159:ALA:HA	1:A:247:MSE:HE1	1.79	0.59
1:B:72:HIS:HD2	1:B:75:SER:HB3	1.68	0.59
1:C:91:GLN:NE2	1:C:92:GLU:N	2.42	0.59
1:D:223:GLU:CD	1:D:223:GLU:H	2.06	0.59
1:A:172:LYS:O	1:A:173:LEU:HD23	2.02	0.58
1:A:142:GLN:HE21	1:A:146:LYS:HE3	1.67	0.58
1:D:303:PRO:CG	1:D:308:LEU:HD13	2.32	0.58
1:A:85:ARG:HA	1:A:205:VAL:HG22	1.84	0.58
1:B:220:MSE:O	1:B:220:MSE:HG2	2.03	0.58
1:D:43:MSE:HB2	1:D:46:PHE:HD2	1.68	0.58
1:B:109:CYS:SG	1:B:110:PRO:CD	2.92	0.58
1:C:72:HIS:ND1	1:C:75:SER:HB3	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ASN:O	1:C:231:GLN:CG	2.44	0.58
1:D:72:HIS:CD2	1:D:74:PRO:HD2	2.39	0.58
1:A:262:THR:HG23	1:A:264:PHE:H	1.69	0.58
1:B:167:GLU:HG3	5:B:364:HOH:O	2.04	0.58
1:A:262:THR:HB	1:A:265:GLN:NE2	2.19	0.57
1:B:109:CYS:SG	1:B:110:PRO:N	2.76	0.57
1:B:121:ARG:NH1	5:B:340:HOH:O	2.37	0.57
1:B:168:HIS:CE1	1:B:172:LYS:HD3	2.40	0.57
1:C:177:HIS:CD2	1:C:179:ASP:CA	2.87	0.57
1:D:54:GLU:OE1	1:D:71:ARG:HD2	2.04	0.57
1:D:217:LYS:CG	1:D:266:GLN:OE1	2.49	0.57
1:B:113:VAL:HG21	1:B:186:LEU:HD22	1.86	0.57
1:A:119:LEU:CD2	1:C:208:VAL:CG1	2.39	0.57
1:A:177:HIS:HE1	1:A:196:CYS:O	1.87	0.56
1:D:231:GLN:O	1:D:232:LYS:HB2	2.05	0.56
1:A:217:LYS:CG	1:A:218:PRO:HD3	2.36	0.56
1:D:46:PHE:CE1	1:D:100:LEU:HD23	2.40	0.56
1:B:134:THR:CG2	5:B:361:HOH:O	2.43	0.56
1:C:55:PRO:CG	1:C:71:ARG:CB	2.78	0.56
1:C:93:GLN:O	1:C:97:LEU:HG	2.06	0.56
1:C:89:ASN:CG	1:C:91:GLN:HG3	2.26	0.56
1:C:220:MSE:H	1:C:220:MSE:SE	2.38	0.56
1:D:95:ARG:HH22	1:D:98:MSE:CE	2.12	0.56
1:B:184:ASN:HD21	1:B:201:SER:H	1.54	0.56
1:B:94:LYS:CE	1:B:98:MSE:HE1	2.35	0.56
1:D:231:GLN:HG2	1:D:232:LYS:CA	2.36	0.56
1:C:291:THR:HG21	5:C:441:HOH:O	1.99	0.56
1:D:43:MSE:C	1:D:44:GLU:HG3	2.25	0.56
1:A:121:ARG:CG	1:C:208:VAL:HG13	2.27	0.55
1:B:169:LEU:HB3	1:B:175:VAL:HB	1.88	0.55
1:C:230:ASN:ND2	5:C:463:HOH:O	2.33	0.55
1:B:229:LEU:HD11	1:D:316:LEU:HB2	1.87	0.55
1:A:303:PRO:HG2	1:A:308:LEU:HD13	1.88	0.55
1:B:94:LYS:HG2	1:B:98:MSE:CE	2.34	0.55
1:C:91:GLN:NE2	1:C:92:GLU:HG3	2.22	0.55
1:B:81:VAL:HG23	1:B:81:VAL:O	2.07	0.55
1:A:303:PRO:CG	1:A:308:LEU:HD13	2.37	0.54
1:C:91:GLN:HE21	1:C:92:GLU:HA	1.69	0.54
1:B:72:HIS:CD2	1:B:75:SER:OG	2.57	0.54
1:A:83:ARG:NH2	1:C:124:ASP:CG	2.60	0.54
1:B:94:LYS:HE2	1:B:98:MSE:HE1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:PRO:HG2	1:C:56:ILE:H	1.72	0.54
1:A:61:ARG:HH12	1:A:66:VAL:N	2.06	0.54
1:B:94:LYS:CE	1:B:98:MSE:CE	2.85	0.54
1:C:240:ILE:HD13	1:C:303:PRO:O	2.07	0.54
1:A:217:LYS:CB	1:A:218:PRO:HD3	2.38	0.54
1:B:248:ILE:HG12	1:B:278:LEU:HD13	1.90	0.54
1:C:119:LEU:HD23	1:C:128:CYS:SG	2.48	0.54
1:C:259:SER:HB3	1:C:266:GLN:CG	2.29	0.54
1:D:298:ASN:HB3	1:D:301:GLU:OE1	2.08	0.53
1:A:289:ASP:O	1:A:293:GLN:HG2	2.08	0.53
1:B:90:SER:O	2:B:4:SO4:O4	2.26	0.53
1:C:91:GLN:HG3	1:C:92:GLU:H	1.73	0.53
1:C:55:PRO:HG2	1:C:71:ARG:H	1.73	0.53
1:B:101:ASP:O	1:B:105:ARG:HG2	2.08	0.53
1:D:137:ASP:O	1:D:141:LYS:HG2	2.09	0.53
1:D:101:ASP:CG	1:D:105:ARG:HH21	2.10	0.53
1:D:105:ARG:HG2	1:D:106:THR:HG23	1.91	0.53
1:C:48:VAL:HG13	1:C:49:LYS:CD	2.33	0.53
1:C:184:ASN:HD21	1:C:201:SER:H	1.57	0.52
1:B:72:HIS:CD2	1:B:75:SER:HB3	2.43	0.52
1:B:89:ASN:OD1	1:B:89:ASN:C	2.48	0.52
1:D:143:VAL:HG13	1:D:148:GLN:HB3	1.91	0.52
1:D:148:GLN:HG3	1:D:149:THR:H	1.73	0.52
1:B:82:LYS:HA	4:B:1:EDO:H22	1.92	0.52
1:C:84:ILE:HD13	1:C:204:LEU:CD1	2.39	0.52
1:C:55:PRO:CG	1:C:71:ARG:H	2.21	0.52
1:D:271:VAL:HG22	1:D:272:GLU:HG3	1.92	0.52
1:A:254:ARG:HD2	5:A:392:HOH:O	2.09	0.52
1:B:317:HIS:HD2	5:B:347:HOH:O	1.93	0.52
1:A:113:VAL:HG21	1:A:186:LEU:CD2	2.37	0.52
1:B:262:THR:CG2	1:B:264:PHE:HB3	2.40	0.52
1:A:326:SER:O	1:A:330:LEU:CD2	2.50	0.51
1:C:149:THR:CG2	1:C:150:ILE:N	2.72	0.51
1:D:109:CYS:SG	1:D:111:PHE:HB2	2.50	0.51
1:B:63:ALA:O	1:B:64:TYR:HB2	2.10	0.51
1:A:309:MSE:HE3	1:A:314:PHE:CZ	2.45	0.51
1:D:131:LEU:C	1:D:131:LEU:HD12	2.29	0.51
1:A:83:ARG:NH2	1:C:124:ASP:OD2	2.29	0.51
1:B:168:HIS:ND1	1:B:172:LYS:HD3	2.25	0.51
1:C:77:GLN:NE2	1:C:116:TYR:CZ	2.79	0.51
1:D:217:LYS:HB3	1:D:218:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TYR:O	1:A:309:MSE:HG3	2.11	0.51
1:B:223:GLU:CD	1:B:223:GLU:H	2.14	0.51
1:D:73:VAL:N	1:D:74:PRO:CD	2.73	0.51
1:D:221:ALA:HB1	1:D:223:GLU:OE2	2.10	0.51
1:B:102:ILE:HD13	1:B:102:ILE:N	2.26	0.51
1:C:248:ILE:HD11	1:C:291:THR:CG2	2.41	0.51
1:C:91:GLN:NE2	1:C:92:GLU:CA	2.66	0.51
1:D:231:GLN:HG2	1:D:232:LYS:O	2.12	0.50
1:B:303:PRO:HG2	1:B:308:LEU:HD13	1.93	0.50
1:C:170:HIS:CD2	1:C:236:VAL:HG11	2.47	0.50
1:D:83:ARG:O	1:D:205:VAL:HG23	2.12	0.50
1:A:153:ASP:OD2	1:A:153:ASP:N	2.45	0.50
1:C:55:PRO:CD	1:C:71:ARG:H	2.24	0.50
1:C:67:VAL:O	1:C:68:GLU:CB	2.51	0.50
1:D:57:MSE:HB2	5:D:401:HOH:O	2.10	0.50
1:A:159:ALA:CB	1:A:247:MSE:HE3	2.42	0.50
1:D:217:LYS:HG3	1:D:218:PRO:HD3	1.93	0.50
1:B:51:ASP:OD1	1:B:51:ASP:O	2.30	0.50
1:A:180:VAL:HG22	1:A:195:MSE:HE1	1.94	0.50
1:B:314:PHE:O	1:B:318:GLU:HB2	2.12	0.50
1:C:263:PRO:HD2	5:C:456:HOH:O	2.11	0.50
1:D:73:VAL:HB	1:D:74:PRO:HD3	1.94	0.50
1:A:305:TYR:HB2	1:A:306:PRO:HD3	1.94	0.49
5:A:364:HOH:O	1:C:129:MSE:SE	2.79	0.49
1:B:93:GLN:HB3	2:B:4:SO4:O3	2.11	0.49
1:C:217:LYS:NZ	1:C:217:LYS:CB	2.74	0.49
1:D:131:LEU:CD1	1:D:132:MSE:N	2.75	0.49
1:D:253:LEU:O	1:D:254:ARG:HB3	2.12	0.49
1:B:248:ILE:CD1	1:B:291:THR:CG2	2.80	0.49
1:C:177:HIS:CD2	1:C:177:HIS:C	2.85	0.49
1:D:154:ILE:HD13	1:D:327:PHE:CG	2.47	0.49
1:B:262:THR:H	1:B:265:GLN:HE21	1.59	0.49
1:C:48:VAL:CG1	1:C:49:LYS:HD3	2.34	0.49
1:B:162:ILE:HG21	1:B:243:LEU:HD13	1.94	0.49
1:B:94:LYS:HE3	1:B:98:MSE:CE	2.42	0.49
1:D:148:GLN:HG3	5:D:439:HOH:O	2.11	0.49
1:A:62:GLY:HA2	1:C:132:MSE:O	2.13	0.49
1:C:55:PRO:O	1:C:56:ILE:CD1	2.60	0.49
1:B:70:MSE:HG2	1:B:81:VAL:HG11	1.95	0.49
1:B:262:THR:HG23	5:B:356:HOH:O	2.11	0.49
1:C:184:ASN:ND2	1:C:201:SER:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:MSE:HB2	1:D:46:PHE:CD2	2.46	0.49
1:D:157:LYS:HE3	1:D:317:HIS:O	2.12	0.49
1:A:262:THR:HG23	5:A:347:HOH:O	2.14	0.48
1:D:217:LYS:CG	1:D:218:PRO:HD3	2.43	0.48
1:D:217:LYS:CB	1:D:218:PRO:HD3	2.43	0.48
1:D:262:THR:CG2	1:D:264:PHE:HB3	2.43	0.48
1:A:237:LYS:HD2	1:A:302:ARG:HB2	1.95	0.48
1:C:134:THR:HG21	1:C:138:LYS:HB2	1.95	0.48
1:C:304:THR:HB	1:C:306:PRO:HD2	1.95	0.48
1:B:94:LYS:CG	1:B:98:MSE:CE	2.91	0.48
1:B:94:LYS:CG	1:B:98:MSE:HE3	2.36	0.48
1:D:56:ILE:HD12	1:D:56:ILE:N	2.27	0.48
1:D:43:MSE:CB	1:D:46:PHE:CD2	2.96	0.48
1:D:72:HIS:CD2	1:D:75:SER:OG	2.67	0.48
1:B:81:VAL:O	1:B:81:VAL:CG2	2.60	0.48
1:B:220:MSE:SE	1:B:220:MSE:H	2.47	0.48
1:B:248:ILE:CG1	1:B:291:THR:HG21	2.43	0.48
1:C:217:LYS:HB3	1:C:218:PRO:CD	2.44	0.48
1:D:121:ARG:NH1	1:D:121:ARG:CG	2.76	0.48
1:A:104:MSE:HE3	1:A:116:TYR:O	2.14	0.48
1:A:262:THR:HG21	1:A:264:PHE:HB3	1.96	0.48
1:C:50:ALA:O	1:C:51:ASP:HB2	2.07	0.48
1:B:72:HIS:CD2	1:B:75:SER:CB	2.91	0.48
1:A:138:LYS:HD3	1:A:138:LYS:N	2.28	0.47
1:B:66:VAL:HG12	1:B:67:VAL:O	2.13	0.47
1:C:279:PRO:HD2	1:C:283:PHE:CE2	2.50	0.47
1:D:298:ASN:OD1	1:D:298:ASN:C	2.53	0.47
1:B:83:ARG:O	4:B:1:EDO:H11	2.14	0.47
1:A:232:LYS:NZ	1:A:232:LYS:CB	2.68	0.47
1:C:89:ASN:OD1	1:C:91:GLN:CG	2.44	0.47
1:C:73:VAL:N	1:C:74:PRO:CD	2.77	0.47
1:D:286:GLU:HA	5:D:455:HOH:O	2.14	0.47
1:A:162:ILE:HD12	1:A:247:MSE:HE2	1.92	0.47
1:D:112:THR:HA	1:D:195:MSE:O	2.14	0.47
1:B:90:SER:HA	2:B:4:SO4:S	2.55	0.47
1:B:168:HIS:O	1:B:172:LYS:HB2	2.14	0.47
1:D:121:ARG:HG3	1:D:121:ARG:NH1	2.27	0.47
1:B:271:VAL:HG22	1:B:272:GLU:HG3	1.95	0.46
1:C:61:ARG:HH11	1:C:61:ARG:HB2	1.80	0.46
1:C:298:ASN:C	1:C:298:ASN:ND2	2.67	0.46
1:C:104:MSE:CG	1:C:115:PHE:O	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:CD	1:A:223:GLU:H	2.17	0.46
1:A:228:GLU:O	1:A:229:LEU:C	2.53	0.46
1:B:177:HIS:O	1:B:178:ARG:HB2	2.16	0.46
1:D:44:GLU:C	1:D:46:PHE:H	2.18	0.46
1:D:95:ARG:HG2	1:D:203:TYR:OH	2.16	0.46
1:D:217:LYS:CB	1:D:218:PRO:CD	2.94	0.46
1:A:320:LYS:HG2	1:A:322:THR:OG1	2.16	0.46
1:D:286:GLU:CD	1:D:286:GLU:H	2.20	0.45
1:C:59:LEU:HG	1:C:60:GLY:N	2.29	0.45
1:D:85:ARG:HA	1:D:205:VAL:HG22	1.97	0.45
1:A:317:HIS:HD2	5:A:349:HOH:O	1.98	0.45
1:D:111:PHE:CE2	1:D:164:LYS:HD3	2.52	0.45
1:A:85:ARG:HG2	1:A:203:TYR:O	2.17	0.45
1:D:224:ARG:HD2	1:D:234:TYR:CD1	2.51	0.45
1:C:48:VAL:CG1	1:C:49:LYS:CD	2.93	0.45
1:C:170:HIS:CD2	1:C:236:VAL:CG1	2.99	0.45
1:A:51:ASP:OD2	1:A:51:ASP:N	2.45	0.45
1:C:195:MSE:HE2	1:C:195:MSE:HB2	1.81	0.45
1:C:84:ILE:HD13	1:C:204:LEU:HD12	1.98	0.44
1:C:55:PRO:CG	1:C:56:ILE:H	2.29	0.44
1:C:206:ASP:O	1:C:207:ASP:HB3	2.14	0.44
1:B:70:MSE:CG	1:B:81:VAL:HG11	2.46	0.44
1:B:268:LYS:HG3	5:B:363:HOH:O	2.16	0.44
1:C:85:ARG:HG2	1:C:203:TYR:O	2.17	0.44
1:B:83:ARG:O	1:B:205:VAL:HG23	2.17	0.44
1:A:142:GLN:NE2	1:A:146:LYS:HE2	2.30	0.44
1:B:85:ARG:HA	1:B:205:VAL:HG22	2.00	0.44
1:B:217:LYS:CB	1:B:218:PRO:CD	2.67	0.44
1:C:79:MSE:HE2	1:C:116:TYR:CG	2.52	0.44
1:A:260:TRP:CE3	1:D:320:LYS:HE3	2.53	0.44
1:D:318:GLU:O	1:D:318:GLU:HG2	2.18	0.44
1:B:305:TYR:HB2	1:B:306:PRO:HD3	2.00	0.43
1:C:220:MSE:HE3	5:C:454:HOH:O	2.17	0.43
1:B:180:VAL:HB	1:B:242:SER:HB2	2.00	0.43
1:B:299:SER:HB3	1:B:302:ARG:CZ	2.48	0.43
1:C:304:THR:CB	1:C:306:PRO:HD2	2.49	0.43
1:C:55:PRO:CD	1:C:71:ARG:N	2.81	0.43
1:C:56:ILE:HG22	1:C:57:MSE:O	2.16	0.43
1:B:170:HIS:O	1:B:174:SER:HA	2.19	0.43
1:B:317:HIS:CD2	5:B:347:HOH:O	2.71	0.43
1:D:232:LYS:HB2	1:D:232:LYS:NZ	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LYS:CD	1:B:266:GLN:OE1	2.60	0.43
1:C:224:ARG:HD3	5:C:462:HOH:O	2.18	0.43
1:C:305:TYR:N	1:C:306:PRO:CD	2.81	0.43
1:D:121:ARG:HH11	1:D:121:ARG:CG	2.23	0.43
1:B:228:GLU:O	1:B:229:LEU:C	2.56	0.43
1:C:148:GLN:OE1	1:C:330:LEU:HD21	2.18	0.43
1:D:92:GLU:HB3	1:D:203:TYR:HE1	1.84	0.43
1:B:142:GLN:O	1:B:146:LYS:HG2	2.19	0.43
1:D:43:MSE:CG	1:D:46:PHE:CD2	2.96	0.43
1:D:154:ILE:HD13	1:D:327:PHE:CD2	2.53	0.43
1:A:309:MSE:HE3	1:A:314:PHE:HZ	1.82	0.43
1:B:52:ASP:O	1:B:53:LEU:CB	2.53	0.43
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.96	0.42
1:B:262:THR:HG23	1:B:264:PHE:H	1.84	0.42
1:A:232:LYS:HB3	1:A:232:LYS:HZ3	1.79	0.42
1:A:173:LEU:O	1:A:174:SER:HB2	2.19	0.42
1:B:258[A]:ASP:CG	1:B:269:GLN:HE22	2.22	0.42
1:A:84:ILE:HD12	1:A:125:VAL:HG12	2.00	0.42
1:B:248:ILE:HD12	1:B:295:LEU:CD1	2.49	0.42
1:D:89:ASN:OD1	1:D:89:ASN:C	2.58	0.42
1:B:79:MSE:HE2	1:B:79:MSE:HB3	1.90	0.42
1:B:105:ARG:HG3	1:B:106:THR:HG23	2.01	0.42
1:D:182:PRO:CD	1:D:246:THR:HB	2.40	0.42
1:D:226:ASN:N	1:D:227:PRO:HD3	2.34	0.42
1:A:258:ASP:HB3	1:A:260:TRP:CZ3	2.55	0.42
1:B:98:MSE:O	1:B:102:ILE:HG12	2.19	0.42
1:B:94:LYS:HA	1:B:97:LEU:HD12	2.02	0.42
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.57	0.42
1:C:50:ALA:HB1	1:C:53:LEU:CD1	2.49	0.42
1:C:152:GLU:OE2	1:C:284:SER:OG	2.36	0.42
1:D:262:THR:HG23	5:D:397:HOH:O	2.20	0.42
1:B:95:ARG:HA	1:B:98:MSE:HG3	2.01	0.42
1:B:240:ILE:HD13	1:B:303:PRO:O	2.19	0.42
1:C:91:GLN:NE2	1:C:92:GLU:HA	2.32	0.42
1:A:298:ASN:HB3	5:A:394:HOH:O	2.20	0.41
1:C:67:VAL:HG12	1:C:69:LYS:H	1.84	0.41
1:C:148:GLN:HG3	1:C:149:THR:H	1.85	0.41
1:D:43:MSE:CB	1:D:46:PHE:HB3	2.45	0.41
1:A:142:GLN:HE21	1:A:146:LYS:CE	2.28	0.41
1:C:55:PRO:HD2	1:C:71:ARG:H	1.84	0.41
1:A:71:ARG:HG2	1:A:78:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ASN:O	1:B:231:GLN:O	2.39	0.41
1:C:262:THR:HB	1:C:263:PRO:CD	2.50	0.41
1:C:278:LEU:HD21	1:C:287:PHE:CE2	2.55	0.41
1:C:307:GLU:O	1:C:310:GLN:HB2	2.20	0.41
1:A:241:TRP:CD1	1:A:241:TRP:C	2.94	0.41
1:C:91:GLN:C	1:C:93:GLN:N	2.73	0.41
1:C:177:HIS:HE1	1:C:196:CYS:O	2.02	0.41
1:A:278:LEU:HD12	1:A:278:LEU:HA	1.79	0.41
1:B:306:PRO:O	1:B:310:GLN:HG2	2.20	0.41
1:C:72:HIS:CE1	1:C:75:SER:HB3	2.55	0.41
1:A:72:HIS:HB2	1:A:79:MSE:HE3	2.01	0.41
1:B:63:ALA:O	1:B:64:TYR:CB	2.69	0.41
1:D:232:LYS:NZ	1:D:232:LYS:CB	2.83	0.41
1:A:217:LYS:HE3	1:A:266:GLN:CD	2.42	0.41
1:C:54:GLU:HA	1:C:55:PRO:HD3	1.84	0.41
1:C:94:LYS:O	1:C:98:MSE:N	2.45	0.41
1:C:142:GLN:O	1:C:146:LYS:HG2	2.21	0.41
1:D:232:LYS:HE2	1:D:232:LYS:HB3	1.80	0.41
1:D:305:TYR:O	1:D:306:PRO:C	2.58	0.41
1:B:298:ASN:OD1	1:B:299:SER:N	2.54	0.40
1:C:72:HIS:ND1	1:C:75:SER:CB	2.85	0.40
1:A:47:GLU:OE2	1:A:120:PHE:CD1	2.69	0.40
1:C:61:ARG:HH11	1:C:61:ARG:CB	2.35	0.40
1:C:149:THR:HG22	1:C:150:ILE:N	2.35	0.40
1:A:146:LYS:O	1:A:147:GLY:C	2.59	0.40
1:B:148:GLN:HG2	5:B:351:HOH:O	2.19	0.40
1:C:48:VAL:CG1	1:C:49:LYS:CG	2.96	0.40
1:D:46:PHE:HD1	1:D:104:MSE:HE1	1.86	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	275/316 (87%)	264 (96%)	10 (4%)	1 (0%)	34 38
1	B	264/316 (84%)	247 (94%)	14 (5%)	3 (1%)	14 13
1	C	269/316 (85%)	244 (91%)	17 (6%)	8 (3%)	4 2
1	D	278/316 (88%)	261 (94%)	14 (5%)	3 (1%)	14 13
All	All	1086/1264 (86%)	1016 (94%)	55 (5%)	15 (1%)	11 9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	GLN
1	C	49	LYS
1	C	51	ASP
1	C	55	PRO
1	C	56	ILE
1	C	107	VAL
1	C	207	ASP
1	A	233	GLY
1	C	174	SER
1	C	284	SER
1	D	44	GLU
1	D	231	GLN
1	D	258	ASP
1	B	60	GLY
1	B	122	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	250/269 (93%)	223 (89%)	27 (11%)	6 6
1	B	245/269 (91%)	214 (87%)	31 (13%)	4 4
1	C	247/269 (92%)	216 (87%)	31 (13%)	4 4
1	D	253/269 (94%)	225 (89%)	28 (11%)	6 5
All	All	995/1076 (92%)	878 (88%)	117 (12%)	5 5

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	54	GLU
1	A	58	GLU
1	A	61	ARG
1	A	98	MSE
1	A	121	ARG
1	A	138	LYS
1	A	149	THR
1	A	153	ASP
1	A	172	LYS
1	A	186	LEU
1	A	204	LEU
1	A	217	LYS
1	A	220	MSE
1	A	223	GLU
1	A	228	GLU
1	A	229	LEU
1	A	231	GLN
1	A	235	SER
1	A	253	LEU
1	A	262	THR
1	A	271	VAL
1	A	278	LEU
1	A	291	THR
1	A	292	SER
1	A	308	LEU
1	A	310	GLN
1	B	51	ASP
1	B	53	LEU
1	B	57	MSE
1	B	58	GLU
1	B	67	VAL
1	B	98	MSE
1	B	102	ILE
1	B	105	ARG
1	B	109	CYS
1	B	121	ARG
1	B	134	THR
1	B	140	TYR
1	B	148	GLN
1	B	167	GLU
1	B	172	LYS

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Mol	Chain	Res	Type
1	B	179	ASP
1	B	186	LEU
1	B	204	LEU
1	B	207	ASP
1	B	217	LYS
1	B	220	MSE
1	B	223	GLU
1	B	224	ARG
1	B	229	LEU
1	B	230	ASN
1	B	231	GLN
1	B	232	LYS
1	B	262	THR
1	B	308	LEU
1	B	318	GLU
1	B	329	LYS
1	C	49	LYS
1	C	57	MSE
1	C	58	GLU
1	C	61	ARG
1	C	69	LYS
1	C	77	GLN
1	C	91	GLN
1	C	93	GLN
1	C	95	ARG
1	C	109	CYS
1	C	119	LEU
1	C	134	THR
1	C	140	TYR
1	C	148	GLN
1	C	179	ASP
1	C	186	LEU
1	C	195	MSE
1	C	204	LEU
1	C	217	LYS
1	C	224	ARG
1	C	229	LEU
1	C	259	SER
1	C	269	GLN
1	C	271	VAL
1	C	281	ASP
1	C	284	SER

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Mol	Chain	Res	Type
1	C	291	THR
1	C	298	ASN
1	C	300	LYS
1	C	310	GLN
1	C	319	SER
1	D	57	MSE
1	D	58	GLU
1	D	59	LEU
1	D	61	ARG
1	D	102	ILE
1	D	105	ARG
1	D	109	CYS
1	D	121	ARG
1	D	131	LEU
1	D	146	LYS
1	D	149	THR
1	D	186	LEU
1	D	197	ASP
1	D	204	LEU
1	D	207	ASP
1	D	217	LYS
1	D	220	MSE
1	D	224	ARG
1	D	229	LEU
1	D	231	GLN
1	D	246	THR
1	D	259	SER
1	D	262	THR
1	D	271	VAL
1	D	278	LEU
1	D	308	LEU
1	D	319	SER
1	D	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	93	GLN
1	A	142	GLN
1	A	170	HIS
1	A	177	HIS

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	230	ASN
1	A	265	GLN
1	B	72	HIS
1	B	93	GLN
1	B	142	GLN
1	B	184	ASN
1	B	265	GLN
1	B	269	GLN
1	B	277	GLN
1	C	77	GLN
1	C	91	GLN
1	C	170	HIS
1	C	177	HIS
1	C	184	ASN
1	C	269	GLN
1	C	298	ASN
1	D	72	HIS
1	D	91	GLN
1	D	93	GLN
1	D	184	ASN
1	D	265	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 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	GOL	A	1	-	5,5,5	0.48	0	5,5,5	0.29	0
2	SO4	B	4	-	4,4,4	0.31	0	6,6,6	0.43	0
2	SO4	A	2	-	4,4,4	0.18	0	6,6,6	0.82	0
2	SO4	D	1	-	4,4,4	0.26	0	6,6,6	1.17	1 (16%)
4	EDO	B	1	-	3,3,3	0.53	0	2,2,2	0.92	0
2	SO4	C	3	-	4,4,4	0.19	0	6,6,6	0.30	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
3	GOL	A	1	-	-	2/4/4/4	-
4	EDO	B	1	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	SO4	O4-S-O3	2.03	117.71	109.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	GOL	C1-C2-C3-O3
3	A	1	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	GOL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	SO4	5	0
2	A	2	SO4	1	0
4	B	1	EDO	7	0
2	C	3	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	268/316 (84%)	0.53	28 (10%) 6 10	47, 56, 67, 73	0
1	B	260/316 (82%)	0.69	37 (14%) 2 4	45, 56, 69, 79	3 (1%)
1	C	264/316 (83%)	0.71	30 (11%) 5 7	42, 57, 68, 76	1 (0%)
1	D	270/316 (85%)	0.79	44 (16%) 1 2	44, 57, 65, 79	0
All	All	1062/1264 (84%)	0.68	139 (13%) 3 5	42, 57, 68, 79	4 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	260	TRP	8.7
1	D	229	LEU	8.3
1	B	105	ARG	6.7
1	A	229	LEU	6.3
1	B	91	GLN	6.2
1	C	62	GLY	5.7
1	D	45	ASN	5.6
1	D	230	ASN	5.6
1	D	233	GLY	5.3
1	D	231	GLN	5.3
1	B	321	GLY	4.6
1	A	232	LYS	4.5
1	D	232	LYS	4.5
1	A	231	GLN	4.5
1	A	230	ASN	4.5
1	B	53	LEU	4.4
1	D	74	PRO	4.3
1	C	231	GLN	4.3
1	C	258	ASP	4.3
1	C	208	VAL	4.2
1	D	44	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	321	GLY	4.0
1	B	50	ALA	4.0
1	D	281	ASP	4.0
1	B	110	PRO	3.9
1	C	230	ASN	3.9
1	C	259	SER	3.9
1	B	95	ARG	3.8
1	B	60	GLY	3.8
1	C	105	ARG	3.8
1	C	300	LYS	3.8
1	B	231	GLN	3.7
1	D	172	LYS	3.6
1	C	59	LEU	3.6
1	A	155	LEU	3.6
1	C	52	ASP	3.5
1	D	291	THR	3.4
1	B	106	THR	3.3
1	C	108	ASP	3.3
1	B	52	ASP	3.3
1	D	295	LEU	3.3
1	A	71	ARG	3.3
1	D	159	ALA	3.2
1	C	279	PRO	3.2
1	D	127	ILE	3.2
1	A	73	VAL	3.2
1	D	294	CYS	3.2
1	C	241	TRP	3.2
1	C	243	LEU	3.2
1	A	244	GLY	3.2
1	D	128	CYS	3.2
1	D	75	SER	3.1
1	B	74	PRO	3.1
1	A	233	GLY	3.1
1	C	244	GLY	3.0
1	D	241	TRP	3.0
1	B	72	HIS	3.0
1	A	321	GLY	3.0
1	D	158	ILE	3.0
1	C	48	VAL	2.9
1	D	282	LYS	2.9
1	A	58	GLU	2.9
1	D	280	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	243	LEU	2.8
1	D	279	PRO	2.8
1	C	58	GLU	2.8
1	D	228	GLU	2.8
1	D	118	ALA	2.8
1	A	319	SER	2.8
1	D	119	LEU	2.7
1	A	74	PRO	2.7
1	D	234	TYR	2.7
1	D	171	SER	2.7
1	D	244	GLY	2.7
1	B	61	ARG	2.6
1	A	174	SER	2.6
1	A	281	ASP	2.5
1	D	162	ILE	2.5
1	B	73	VAL	2.5
1	C	281	ASP	2.5
1	C	97	LEU	2.5
1	A	115	PHE	2.5
1	D	243	LEU	2.5
1	B	319	SER	2.4
1	B	281	ASP	2.4
1	D	63	ALA	2.4
1	A	76	GLY	2.4
1	B	259	SER	2.4
1	B	155	LEU	2.4
1	D	59	LEU	2.4
1	A	91	GLN	2.4
1	B	222	PRO	2.4
1	C	187	ILE	2.4
1	A	154	ILE	2.4
1	B	241	TRP	2.4
1	D	108	ASP	2.4
1	A	259	SER	2.4
1	B	230	ASN	2.4
1	A	240	ILE	2.3
1	A	248	ILE	2.3
1	B	243	LEU	2.3
1	B	200	ILE	2.3
1	D	77	GLN	2.3
1	D	73	VAL	2.3
1	D	301	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	298	ASN	2.3
1	B	159	ALA	2.3
1	C	159	ALA	2.3
1	C	172	LYS	2.3
1	D	51	ASP	2.3
1	B	240	ILE	2.3
1	D	245	ILE	2.3
1	D	91	GLN	2.3
1	B	308	LEU	2.2
1	C	204	LEU	2.2
1	B	158	ILE	2.2
1	B	300	LYS	2.2
1	B	101	ASP	2.2
1	C	158	ILE	2.2
1	C	162	ILE	2.2
1	B	108	ASP	2.2
1	A	298	ASN	2.2
1	A	158	ILE	2.2
1	C	294	CYS	2.2
1	A	196	CYS	2.1
1	B	250	LEU	2.1
1	D	290	PHE	2.1
1	B	174	SER	2.1
1	C	240	ILE	2.1
1	A	308	LEU	2.1
1	B	90	SER	2.1
1	B	175	VAL	2.1
1	C	282	LYS	2.1
1	D	62	GLY	2.1
1	A	260	TRP	2.1
1	B	150	ILE	2.0
1	B	80	ALA	2.0
1	C	150	ILE	2.0
1	D	248	ILE	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	GOL	A	1	6/6	0.76	0.41	66,73,75,75	0
2	SO4	B	4	5/5	0.81	0.30	125,125,126,127	0
4	EDO	B	1	4/4	0.93	0.49	49,49,54,56	0
2	SO4	C	3	5/5	0.95	0.31	97,97,99,99	0
2	SO4	D	1	5/5	0.96	0.22	72,73,74,74	0
2	SO4	A	2	5/5	0.98	0.18	64,66,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.