



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:29 AM UTC

PDB ID : 7OX2 / pdb_00007ox2
Title : Fab 6E2: hIL-9 complex
Authors : De Vos, T.; Savvides, S.N.
Deposited on : 2021-06-22
Resolution : 3.34 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

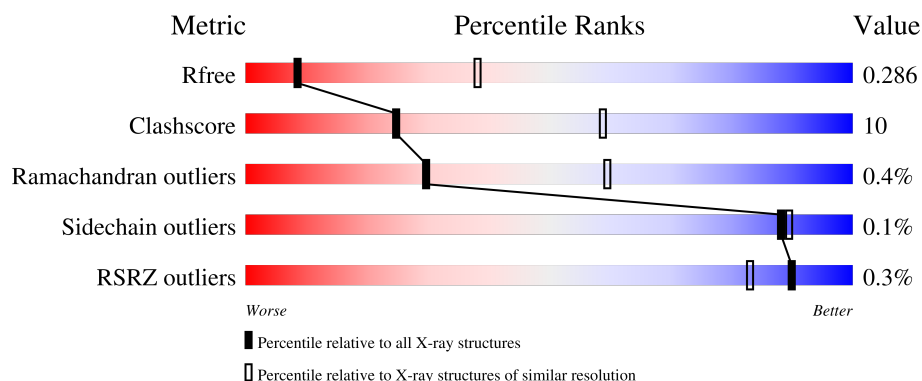
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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 $\leq 5\%$. 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	220	81% 15% .
1	B	220	78% 19% .
1	D	220	79% 16% 5%
1	J	220	74% 21% 5%
2	C	214	86% 13% .

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Mol	Chain	Length	Quality of chain
2	E	214	78%20%•
2	K	214	77%21%•
2	L	214	79%19%•
3	M	130	2% 70%22%8%
3	N	130	2% 65%26%8%
3	O	130	% 67%18%•15%
3	T	130	68%20%•10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31936 atoms, of which 15777 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 Heavy chain (Fab 6E2).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	212	Total	C	H	N	O	S	0	0	0
			3109	995	1539	256	314	5			
1	B	213	Total	C	H	N	O	S	0	0	0
			3121	998	1545	257	316	5			
1	D	210	Total	C	H	N	O	S	0	0	0
			3091	990	1531	254	311	5			
1	J	210	Total	C	H	N	O	S	0	0	0
			3085	988	1528	253	311	5			

- Molecule 2 is a protein called Light chain (Fab 6E2).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	209	Total	C	H	N	O	S	0	0	0
			3050	966	1493	263	324	4			
2	C	210	Total	C	H	N	O	S	0	0	0
			3060	969	1497	264	326	4			
2	E	209	Total	C	H	N	O	S	0	0	0
			3049	966	1492	263	324	4			
2	K	209	Total	C	H	N	O	S	0	0	0
			3048	966	1491	263	324	4			

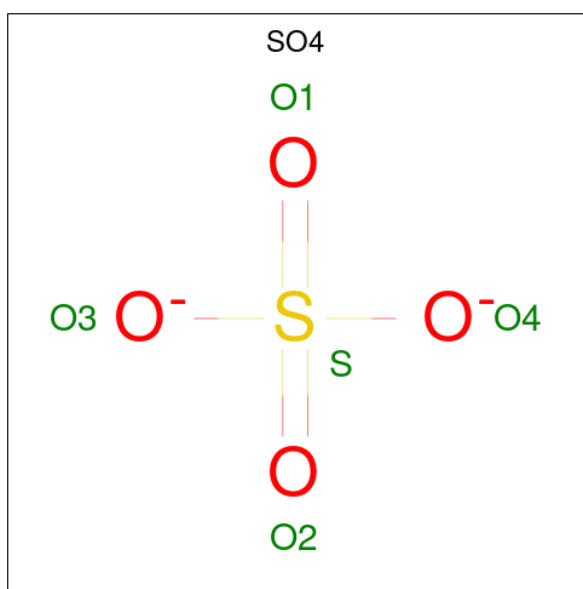
- Molecule 3 is a protein called Interleukin-9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	T	117	Total	C	H	N	O	S	0	0	0
			1832	571	918	158	172	13			
3	O	111	Total	C	H	N	O	S	0	0	0
			1753	548	884	149	160	12			
3	M	120	Total	C	H	N	O	S	0	0	0
			1859	578	931	161	175	14			
3	N	119	Total	C	H	N	O	S	0	0	0
			1852	576	928	160	174	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	15	GLY	-	expression tag	UNP P15248
T	16	SER	-	expression tag	UNP P15248
T	17	HIS	-	expression tag	UNP P15248
T	18	MET	-	expression tag	UNP P15248
O	15	GLY	-	expression tag	UNP P15248
O	16	SER	-	expression tag	UNP P15248
O	17	HIS	-	expression tag	UNP P15248
O	18	MET	-	expression tag	UNP P15248
M	15	GLY	-	expression tag	UNP P15248
M	16	SER	-	expression tag	UNP P15248
M	17	HIS	-	expression tag	UNP P15248
M	18	MET	-	expression tag	UNP P15248
N	15	GLY	-	expression tag	UNP P15248
N	16	SER	-	expression tag	UNP P15248
N	17	HIS	-	expression tag	UNP P15248
N	18	MET	-	expression tag	UNP P15248

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		

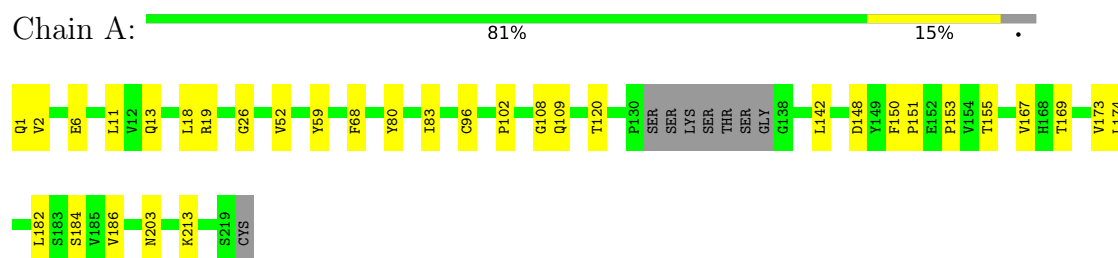
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		

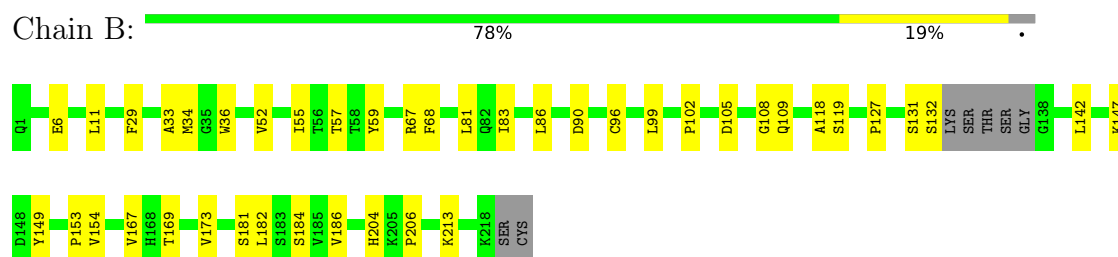
3 Residue-property plots

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.

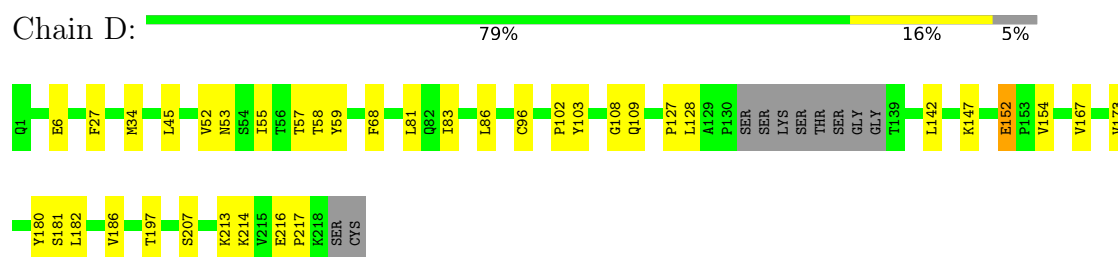
- Molecule 1: Heavy chain (Fab 6E2)



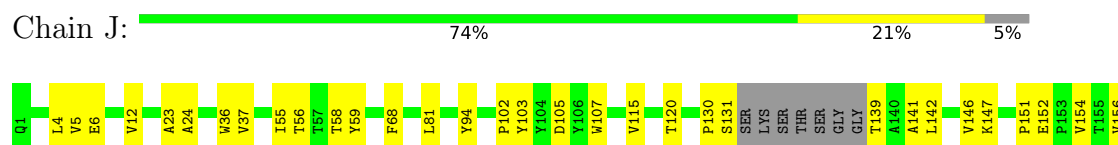
- Molecule 1: Heavy chain (Fab 6E2)



- Molecule 1: Heavy chain (Fab 6E2)



- Molecule 1: Heavy chain (Fab 6E2)





• Molecule 2: Light chain (Fab 6E2)

Chain L: 79% 19%



• Molecule 2: Light chain (Fab 6E2)

Chain C: 86% 13%



• Molecule 2: Light chain (Fab 6E2)

Chain E: 78% 20%



• Molecule 2: Light chain (Fab 6E2)

Chain K: 77% 21%



• Molecule 3: Interleukin-9

Chain T: 68% 20% 10%



R138
GLY
MET
ARG
GLY
LYS
ILE

• Molecule 3: Interleukin-9



GLY SER HIS MET MET GLN GLY C21 L24 I27 L33 M37 C47 V51 L55 C56 L57 P60 SER ASP ASN CYS T65 R66 P67 R72 M76 T79 T80 M81 R84 I88 Q111 P112 CYS ASN GLN T116 T117 A118 L125 L128 I131 F132

Q133
GLY
MET
ARG
GLY
LYS
ILE

• Molecule 3: Interleukin-9



GLY SER HIS MET MET GLN G20 L24 A25 G26 I27 N31 F32 L33 I34 N35 N36 M37 Q38 S48 V51 L73 M76 T77 N78 T79 T80 M81 Q82 L87 E97 C109 E110 Q111 A118 F124 L128 I131 F132 E135 K136 M137 R138 G139 MET ARG GLY

LYS
ILE

• Molecule 3: Interleukin-9



GLY SER HIS MET MET GLN G20 L24 I27 N31 F32 L33 I34 M37 H46 C47 S48 A49 N50 V51 S61 D62 N63 C64 T65 R66 R72 T77 N78 M81 Q82 T83 R84 Y85 I88 R91 E110 C113 T116 T117 A118 L128 I131 F132 Q133

K136
M137
R138
GLY
MET
ARG
GLY
LYS
ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.36Å 94.36Å 107.33Å 82.54° 72.00° 80.79°	Depositor
Resolution (Å)	48.92 – 3.34 48.92 – 3.34	Depositor EDS
% Data completeness (in resolution range)	93.6 (48.92-3.34) 93.5 (48.92-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.224 , 0.283 0.225 , 0.286	Depositor DCC
R_{free} test set	1732 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31936	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/1607	0.50	0/2194
1	B	0.17	0/1613	0.43	0/2202
1	D	0.16	0/1597	0.45	0/2181
1	J	0.26	0/1593	0.62	4/2174 (0.2%)
2	C	0.19	0/1599	0.51	0/2186
2	E	0.16	0/1593	0.45	0/2178
2	K	0.23	0/1593	0.52	0/2178
2	L	0.23	0/1593	0.53	0/2178
3	M	0.35	0/943	0.92	2/1271 (0.2%)
3	N	0.32	0/939	0.94	6/1266 (0.5%)
3	O	0.31	0/882	0.90	2/1186 (0.2%)
3	T	0.32	0/928	0.82	0/1250
All	All	0.24	0/16480	0.61	14/22444 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	47	CYS	N-CA-C	-8.49	103.36	114.31
3	O	47	CYS	N-CA-C	-7.80	104.24	114.31
3	N	46	HIS	CA-C-N	6.54	132.50	122.24
3	N	46	HIS	C-N-CA	6.54	132.50	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	152	GLU	CA-C-N	5.92	141.21	127.00
1	J	152	GLU	C-N-CA	5.92	141.21	127.00
3	O	67	PRO	N-CA-C	5.92	121.25	113.86
1	J	197	THR	N-CA-C	5.70	118.39	108.76
1	J	152	GLU	C-N-CD	-5.44	108.64	120.60
3	M	78	ASN	CB-CA-C	-5.27	102.45	111.26
3	M	110	GLU	CA-CB-CG	-5.27	103.56	114.10
3	N	50	ASN	N-CA-C	-5.14	104.33	111.52
3	N	82	GLN	CA-C-N	-5.01	112.16	120.68
3	N	82	GLN	C-N-CA	-5.01	112.16	120.68

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	152	GLU	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	1570	1539	1539	31	0
1	B	1576	1545	1544	38	2
1	D	1560	1531	1531	34	1
1	J	1557	1528	1527	33	1
2	C	1563	1497	1497	19	1
2	E	1557	1492	1492	36	0
2	K	1557	1491	1492	35	1
2	L	1557	1493	1492	33	2
3	M	928	931	931	28	0
3	N	924	928	928	27	0
3	O	869	884	884	29	0
3	T	914	918	919	27	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
4	D	5	0	0	0	0
4	M	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	L	1	0	0	0	0
All	All	16159	15777	15776	313	4

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 10.

All (313) 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:57:THR:OG1	3:O:133:GLN:OE1	1.67	1.12
3:M:111:GLN:OE1	2:K:66:SER:OG	1.68	1.10
1:J:58:THR:O	3:N:136:LYS:NZ	1.86	1.07
3:O:76:MET:HE3	3:O:79:THR:HG21	1.44	0.97
1:D:58:THR:O	3:M:136:LYS:NZ	1.98	0.96
3:N:66:ARG:NH2	3:N:113:CYS:SG	2.41	0.93
1:J:147:LYS:O	1:J:181:SER:OG	1.89	0.89
3:T:64:CYS:O	3:T:65:THR:OG1	1.90	0.88
3:O:51:VAL:HG21	3:N:118:ALA:HB2	1.57	0.84
1:D:59:TYR:CG	3:M:24:LEU:HD12	2.16	0.81
2:K:31:ASP:O	2:K:89:SER:OG	1.99	0.80
2:K:53:ARG:HG2	2:K:57:ILE:HD11	1.62	0.79
2:E:147:THR:HG1	2:E:198:THR:HG1	1.30	0.78
1:D:147:LYS:O	1:D:181:SER:OG	2.03	0.74
1:B:55:ILE:HD13	3:O:133:GLN:HG3	1.70	0.74
1:B:147:LYS:O	1:B:181:SER:OG	2.04	0.73
2:E:23:GLN:HB3	2:E:69:THR:HG22	1.70	0.73
1:J:59:TYR:CG	3:N:24:LEU:HD12	2.25	0.72
3:O:88:ILE:HD12	3:O:88:ILE:H	1.54	0.71
2:K:33:HIS:ND1	2:K:48:HIS:O	2.22	0.71
3:N:88:ILE:HD12	3:N:88:ILE:H	1.57	0.70
3:T:51:VAL:HG21	3:M:118:ALA:HB2	1.72	0.70
1:D:59:TYR:OH	3:M:27:ILE:HD12	1.91	0.70
2:L:49:ASP:OD2	3:T:91:ARG:NH2	2.25	0.70
2:K:169:GLN:HG2	2:K:170:SER:H	1.57	0.69
3:M:128:LEU:O	3:M:131:ILE:HG22	1.92	0.69
2:C:147:THR:HG1	2:C:198:THR:HG1	1.39	0.68
3:T:66:ARG:NH1	3:T:111:GLN:O	2.26	0.68
1:J:120:THR:HG23	1:J:151:PRO:HD2	1.77	0.67
3:M:76:MET:HE1	3:M:124:PHE:CE2	2.30	0.66
1:A:68:PHE:CD1	1:A:83:ILE:HG22	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LYS:NZ	2:L:125:GLU:OE1	2.17	0.66
2:C:50:ASN:OD1	2:C:51:ASN:N	2.29	0.65
1:J:102:PRO:O	2:K:88:GLN:NE2	2.30	0.65
1:B:55:ILE:HG21	3:O:133:GLN:HG3	1.79	0.64
1:D:102:PRO:O	2:E:88:GLN:NE2	2.29	0.64
2:E:67:GLY:HA3	3:N:110:GLU:O	1.98	0.64
1:B:173:VAL:HG22	2:C:164:THR:CG2	2.28	0.63
2:K:27:LEU:O	2:K:65:ARG:NH1	2.31	0.63
3:O:76:MET:CE	3:O:79:THR:HG21	2.24	0.63
1:J:139:THR:HA	1:J:189:PRO:HA	1.81	0.63
1:A:169:THR:HG23	1:A:184:SER:HB3	1.81	0.63
3:T:81:MET:HE1	3:T:121:ALA:HB1	1.80	0.63
2:L:57:ILE:HD12	2:L:57:ILE:C	2.25	0.62
1:J:173:VAL:HG22	2:K:164:THR:HG22	1.81	0.62
1:D:173:VAL:HG22	2:E:164:THR:CG2	2.29	0.62
2:E:23:GLN:CB	2:E:69:THR:HG22	2.29	0.61
2:E:47:ILE:HD12	2:E:72:LEU:CD1	2.31	0.61
3:M:111:GLN:OE1	2:K:66:SER:CB	2.48	0.60
2:E:53:ARG:HG2	2:E:57:ILE:HD11	1.83	0.60
1:A:167:VAL:HG22	1:A:186:VAL:HG12	1.82	0.60
1:B:55:ILE:HG21	3:O:133:GLN:CD	2.27	0.59
2:L:152:ALA:HB2	2:L:193:TYR:CE2	2.37	0.59
1:A:102:PRO:O	2:L:88:GLN:NE2	2.35	0.59
1:J:173:VAL:HG22	2:K:164:THR:CG2	2.33	0.59
2:L:147:THR:OG1	2:L:198:THR:OG1	2.12	0.59
1:B:102:PRO:O	2:C:88:GLN:NE2	2.35	0.58
1:J:59:TYR:OH	3:N:27:ILE:HD12	2.03	0.58
1:A:174:LEU:HD23	1:A:174:LEU:O	2.03	0.58
1:A:59:TYR:OH	3:T:27:ILE:HD12	2.04	0.58
1:A:96:CYS:O	1:A:108:GLY:N	2.37	0.58
2:C:23:GLN:HB3	2:C:69:THR:HG22	1.84	0.58
2:K:26:SER:HB3	2:K:90:TYR:O	2.03	0.58
2:L:4:LEU:HD13	2:L:22:CYS:SG	2.44	0.57
3:T:62:ASP:OD1	3:T:62:ASP:N	2.36	0.57
2:K:27:LEU:HD22	2:K:32:ALA:HB2	1.86	0.57
3:N:85:TYR:HB3	3:N:88:ILE:HD13	1.85	0.57
1:A:142:LEU:HD12	1:A:142:LEU:C	2.30	0.57
3:T:90:SER:O	3:T:94:LYS:HD3	2.05	0.57
3:T:60:PRO:HG2	3:T:69:PHE:CZ	2.40	0.56
1:B:182:LEU:C	1:B:182:LEU:HD12	2.30	0.56
2:L:57:ILE:HD12	2:L:58:PRO:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:VAL:HG22	2:E:164:THR:HG23	1.86	0.56
1:B:59:TYR:OH	3:O:27:ILE:HD12	2.05	0.56
1:D:55:ILE:HD13	1:D:57:THR:OG1	2.06	0.56
2:L:53:ARG:HD3	2:L:57:ILE:HD11	1.86	0.56
3:T:76:MET:HG3	3:T:82:GLN:HE22	1.70	0.55
2:E:110:GLN:HB2	2:E:142:TYR:CZ	2.42	0.55
1:A:18:LEU:HD11	1:A:83:ILE:HD11	1.87	0.55
3:T:63:ASN:O	3:T:65:THR:N	2.40	0.55
3:N:31:ASN:HD22	3:N:31:ASN:C	2.14	0.55
2:L:35:TYR:HE2	2:L:88:GLN:HG2	1.72	0.55
3:T:81:MET:O	3:T:84:ARG:O	2.25	0.55
1:B:173:VAL:HG22	2:C:164:THR:HG22	1.88	0.55
1:D:182:LEU:C	1:D:182:LEU:HD12	2.32	0.55
3:M:79:THR:OG1	3:M:81:MET:HE3	2.07	0.55
2:C:53:ARG:HG2	2:C:57:ILE:HD11	1.88	0.54
1:A:120:THR:HG23	1:A:151:PRO:HD3	1.89	0.54
2:C:53:ARG:HD3	2:C:61:PHE:O	2.08	0.54
3:T:61:SER:OG	3:T:62:ASP:N	2.41	0.54
2:K:168:LYS:HG3	2:K:174:TYR:CE1	2.42	0.54
1:J:59:TYR:CD2	3:N:24:LEU:HD12	2.43	0.54
1:B:96:CYS:O	1:B:108:GLY:N	2.42	0.53
3:N:63:ASN:O	3:N:65:THR:HG23	2.08	0.53
2:E:53:ARG:HD3	2:E:61:PHE:O	2.07	0.53
2:K:31:ASP:OD2	3:N:91:ARG:NE	2.36	0.53
1:B:68:PHE:CD1	1:B:83:ILE:HG22	2.44	0.53
1:D:167:VAL:HG22	1:D:186:VAL:HG12	1.90	0.53
1:J:182:LEU:HD12	1:J:182:LEU:C	2.33	0.53
2:K:110:GLN:NE2	2:K:172:ASN:OD1	2.37	0.53
2:K:151:LYS:HA	2:K:155:SER:O	2.08	0.53
1:D:6:GLU:OE2	1:D:109:GLN:N	2.42	0.53
2:L:35:TYR:CE2	2:L:88:GLN:HG2	2.44	0.52
1:B:55:ILE:HG21	3:O:133:GLN:CG	2.39	0.52
3:O:66:ARG:NH1	3:O:111:GLN:NE2	2.57	0.52
1:D:216:GLU:HG3	1:D:217:PRO:HD2	1.90	0.52
1:J:195:THR:C	1:J:197:THR:N	2.68	0.52
3:N:88:ILE:HD12	3:N:88:ILE:N	2.22	0.52
1:B:154:VAL:HG22	1:B:182:LEU:HD21	1.92	0.52
1:J:55:ILE:HG13	1:J:55:ILE:O	2.10	0.52
3:M:76:MET:HE1	3:M:124:PHE:CZ	2.45	0.51
2:E:27:LEU:HD22	2:E:32:ALA:HB2	1.91	0.51
1:D:68:PHE:CD1	1:D:83:ILE:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:ASP:HB3	2:L:50:ASN:OD1	2.11	0.51
1:B:173:VAL:HG22	2:C:164:THR:HG23	1.92	0.51
1:J:131:SER:O	1:J:131:SER:OG	2.27	0.51
1:A:182:LEU:C	1:A:182:LEU:HD12	2.35	0.51
1:D:197:THR:HG23	1:D:214:LYS:CE	2.41	0.51
1:A:1:GLN:OE1	1:A:2:VAL:HG22	2.11	0.51
2:C:142:TYR:HB3	2:C:143:PRO:HD3	1.93	0.51
3:O:88:ILE:HD12	3:O:88:ILE:N	2.23	0.51
3:N:81:MET:O	3:N:84:ARG:O	2.28	0.51
1:D:154:VAL:HG22	1:D:182:LEU:HD21	1.93	0.51
2:E:194:SER:CB	2:E:207:THR:HG22	2.40	0.50
1:A:68:PHE:CG	1:A:83:ILE:HG22	2.46	0.50
2:L:53:ARG:HD3	2:L:57:ILE:CD1	2.41	0.50
2:L:114:ALA:O	2:L:140:ASP:O	2.29	0.50
2:E:31:ASP:OD2	3:M:87:LEU:HD21	2.12	0.50
2:L:168:LYS:HG3	2:L:174:TYR:HE1	1.76	0.50
1:J:56:THR:O	1:J:56:THR:OG1	2.26	0.50
3:T:76:MET:HG3	3:T:82:GLN:NE2	2.25	0.50
1:B:11:LEU:HD21	1:B:118:ALA:O	2.11	0.50
1:B:52:VAL:HG21	3:O:27:ILE:CG2	2.42	0.50
3:N:31:ASN:HA	3:N:34:ILE:HG12	1.94	0.50
1:A:173:VAL:HG22	2:L:164:THR:CG2	2.42	0.50
1:B:68:PHE:CG	1:B:83:ILE:HG22	2.47	0.50
3:M:73:LEU:HD23	3:M:76:MET:HE3	1.93	0.50
2:K:23:GLN:HB2	2:K:69:THR:HG22	1.94	0.49
1:A:11:LEU:C	1:A:11:LEU:HD23	2.38	0.49
1:B:29:PHE:N	4:B:301:SO4:O3	2.45	0.49
1:D:59:TYR:CD1	3:M:24:LEU:HD12	2.47	0.49
3:M:27:ILE:CG1	3:M:132:PHE:HB3	2.42	0.49
3:M:31:ASN:HA	3:M:34:ILE:HG12	1.95	0.49
1:D:96:CYS:O	1:D:108:GLY:N	2.44	0.49
1:D:103:TYR:HA	2:E:88:GLN:NE2	2.28	0.49
3:N:88:ILE:H	3:N:88:ILE:CD1	2.25	0.49
1:D:52:VAL:HG13	3:M:31:ASN:HD22	1.78	0.49
3:M:135:GLU:O	3:M:138:ARG:NE	2.40	0.49
3:M:48:SER:OG	4:M:201:SO4:S	2.70	0.48
2:L:82:GLU:HG3	2:L:105:LEU:O	2.13	0.48
3:N:64:CYS:O	3:N:65:THR:OG1	2.20	0.48
1:A:6:GLU:OE2	1:A:109:GLN:N	2.46	0.48
2:L:12:VAL:HG12	2:L:105:LEU:HD11	1.95	0.48
1:A:155:THR:HG22	1:A:203:ASN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:82:GLN:HB3	3:N:77:THR:OG1	2.13	0.48
1:J:4:LEU:HD23	1:J:24:ALA:HB2	1.96	0.48
2:L:168:LYS:HG3	2:L:174:TYR:CE1	2.49	0.48
2:E:90:TYR:CG	3:M:25:ALA:HB2	2.49	0.48
1:J:130:PRO:HB3	1:J:141:ALA:O	2.14	0.48
2:E:21:THR:HG22	2:E:71:THR:HG22	1.96	0.48
2:K:141:PHE:O	2:K:174:TYR:HB2	2.14	0.48
1:B:167:VAL:HG22	1:B:186:VAL:HG12	1.96	0.47
3:O:81:MET:HE3	3:O:125:LEU:HD21	1.96	0.47
2:E:121:PRO:HA	2:E:134:LEU:HD23	1.96	0.47
1:J:156:VAL:HG22	1:J:202:VAL:HG22	1.96	0.47
3:T:81:MET:CE	3:T:121:ALA:HB1	2.44	0.47
2:C:109:GLY:O	2:C:111:PRO:HD3	2.15	0.47
3:T:76:MET:HE1	3:T:124:PHE:CZ	2.50	0.47
1:D:173:VAL:HG22	2:E:164:THR:HG22	1.95	0.47
1:D:167:VAL:HG13	1:D:186:VAL:HG12	1.97	0.47
3:N:128:LEU:O	3:N:131:ILE:HG22	2.15	0.47
3:M:79:THR:HG23	3:M:81:MET:HG2	1.95	0.47
3:N:77:THR:HG22	3:N:78:ASN:OD1	2.14	0.47
2:E:82:GLU:HG3	2:E:106:THR:HA	1.96	0.46
3:T:35:ASN:O	3:T:38:GLN:HG2	2.16	0.46
3:T:128:LEU:O	3:T:131:ILE:HG22	2.15	0.46
1:J:154:VAL:HG12	1:J:204:HIS:HB2	1.96	0.46
2:K:31:ASP:HB3	2:K:50:ASN:OD1	2.15	0.46
1:B:127:PRO:HD3	1:B:213:LYS:HE2	1.98	0.46
3:O:128:LEU:O	3:O:131:ILE:HG22	2.15	0.46
2:E:20:ILE:HG23	2:E:103:THR:HG21	1.97	0.46
1:D:127:PRO:HD3	1:D:213:LYS:HE2	1.98	0.46
2:L:141:PHE:O	2:L:174:TYR:HB2	2.16	0.46
1:A:18:LEU:C	1:A:18:LEU:HD12	2.40	0.46
3:T:77:THR:HA	3:T:82:GLN:OE1	2.15	0.46
2:E:169:GLN:CD	2:E:175:ALA:HB2	2.41	0.46
3:T:64:CYS:O	3:T:65:THR:CB	2.63	0.46
1:B:52:VAL:HG21	3:O:27:ILE:HG22	1.98	0.46
2:K:143:PRO:HG2	2:K:199:HIS:CE1	2.50	0.46
1:A:167:VAL:HG22	1:A:186:VAL:CG1	2.45	0.46
2:L:60:ARG:HD2	2:L:75:SER:O	2.16	0.46
2:L:135:VAL:HG13	2:L:179:TYR:HE1	1.79	0.45
1:A:1:GLN:OE1	1:A:26:GLY:CA	2.64	0.45
2:E:110:GLN:HB2	2:E:142:TYR:CE1	2.50	0.45
1:A:173:VAL:HG23	2:L:179:TYR:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:66:ARG:HH12	3:O:111:GLN:NE2	2.14	0.45
2:C:35:TYR:HE2	2:C:88:GLN:HG2	1.81	0.45
1:J:105:ASP:HA	2:K:45:LEU:HD22	1.98	0.45
2:K:110:GLN:HB2	2:K:111:PRO:HD2	1.99	0.45
1:A:19:ARG:NH2	1:A:80:TYR:CZ	2.84	0.45
2:L:60:ARG:HH21	2:L:81:ASP:CG	2.25	0.45
1:D:45:LEU:HD12	2:E:86:TYR:CG	2.52	0.44
1:D:142:LEU:C	1:D:142:LEU:HD12	2.42	0.44
2:L:169:GLN:OE1	2:L:175:ALA:HB2	2.17	0.44
3:O:72:ARG:NH2	3:O:116:THR:HG21	2.33	0.44
1:J:36:TRP:CD1	1:J:81:LEU:HD13	2.52	0.44
2:K:53:ARG:CG	2:K:57:ILE:HD11	2.41	0.44
1:A:13:GLN:OE1	1:A:13:GLN:N	2.48	0.44
1:B:55:ILE:CG2	3:O:133:GLN:CD	2.90	0.44
2:K:14:LEU:HD12	2:K:107:VAL:HG11	1.98	0.44
2:K:53:ARG:HD3	2:K:61:PHE:O	2.18	0.44
2:E:194:SER:HB3	2:E:207:THR:HG22	1.99	0.44
2:C:23:GLN:CB	2:C:69:THR:HG22	2.48	0.44
1:J:5:VAL:HG22	1:J:23:ALA:HB3	1.99	0.44
1:A:169:THR:HG23	1:A:184:SER:CB	2.48	0.44
1:B:57:THR:OG1	3:O:133:GLN:CD	2.55	0.44
3:O:118:ALA:HB2	3:N:51:VAL:HG21	1.99	0.44
1:J:6:GLU:OE1	1:J:94:TYR:O	2.36	0.44
1:J:146:VAL:HG22	1:J:202:VAL:HG21	1.99	0.44
1:A:68:PHE:CD1	1:A:68:PHE:N	2.86	0.43
2:L:135:VAL:HG13	2:L:179:TYR:CE1	2.52	0.43
1:B:142:LEU:C	1:B:142:LEU:HD12	2.43	0.43
1:D:27:PHE:CZ	1:D:34:MET:HE3	2.53	0.43
1:J:142:LEU:HD12	1:J:142:LEU:C	2.43	0.43
2:K:61:PHE:CE2	2:K:74:ILE:HG12	2.52	0.43
1:B:169:THR:HG23	1:B:184:SER:HB3	2.00	0.43
1:D:216:GLU:HG3	1:D:217:PRO:CD	2.48	0.43
3:M:97:GLU:OE2	4:M:202:SO4:O1	2.37	0.43
2:C:82:GLU:HG3	2:C:106:THR:HA	1.99	0.43
3:M:33:LEU:O	3:M:37:MET:HG2	2.19	0.43
3:O:88:ILE:H	3:O:88:ILE:CD1	2.24	0.43
3:N:33:LEU:O	3:N:37:MET:HG2	2.19	0.43
3:T:118:ALA:HB2	3:M:51:VAL:HG21	2.00	0.43
1:D:128:LEU:HB3	2:E:120:PHE:CD2	2.54	0.43
2:L:142:TYR:HB3	2:L:143:PRO:HD3	2.00	0.43
2:C:121:PRO:HA	2:C:134:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:79:THR:CG2	3:M:81:MET:HG2	2.49	0.43
2:C:187:TRP:CZ2	2:C:210:PRO:HA	2.54	0.43
2:K:20:ILE:HG23	2:K:103:THR:HG21	1.99	0.43
2:E:38:LYS:HE2	2:E:80:GLU:O	2.19	0.43
3:O:60:PRO:CG	3:O:67:PRO:HB3	2.49	0.43
3:M:136:LYS:O	3:M:136:LYS:HG2	2.18	0.43
3:N:72:ARG:NH2	3:N:116:THR:HG21	2.34	0.43
1:B:6:GLU:OE2	1:B:109:GLN:N	2.48	0.42
2:K:143:PRO:HG2	2:K:199:HIS:HE1	1.84	0.42
1:D:173:VAL:O	1:D:180:TYR:HA	2.20	0.42
1:A:142:LEU:HD12	1:A:142:LEU:O	2.20	0.42
1:B:83:ILE:HD12	1:B:86:LEU:HD21	2.00	0.42
2:C:110:GLN:O	2:C:110:GLN:HG2	2.19	0.42
1:J:55:ILE:HG21	3:N:133:GLN:OE1	2.19	0.42
1:A:52:VAL:HG21	3:T:27:ILE:CG2	2.49	0.42
1:D:81:LEU:HD23	1:D:83:ILE:HG23	2.01	0.42
1:J:55:ILE:O	1:J:55:ILE:HG23	2.20	0.42
1:A:1:GLN:OE1	1:A:26:GLY:O	2.38	0.42
2:L:49:ASP:OD2	3:T:91:ARG:CZ	2.68	0.42
1:B:131:SER:O	1:B:132:SER:C	2.63	0.42
1:D:167:VAL:HG22	1:D:186:VAL:CG1	2.49	0.42
2:E:35:TYR:HE2	2:E:88:GLN:HG2	1.84	0.42
3:N:84:ARG:HG2	3:N:85:TYR:CE2	2.54	0.42
2:L:27:LEU:HD22	2:L:32:ALA:HB2	2.02	0.42
1:J:103:TYR:HA	2:K:88:GLN:NE2	2.35	0.42
1:B:36:TRP:CG	1:B:81:LEU:HD13	2.55	0.42
2:C:59:GLU:OE1	2:C:59:GLU:N	2.53	0.42
2:E:59:GLU:CD	2:E:59:GLU:H	2.28	0.42
2:L:84:ASP:OD1	2:L:104:GLN:HG2	2.20	0.42
3:O:66:ARG:N	3:O:67:PRO:CD	2.83	0.42
3:N:65:THR:C	3:N:66:ARG:HG3	2.44	0.42
1:B:204:HIS:HE1	1:B:206:PRO:HB2	1.85	0.42
1:J:12:VAL:HG23	1:J:115:VAL:HG22	2.01	0.42
2:L:127:LEU:HD23	2:L:127:LEU:HA	1.89	0.41
1:B:81:LEU:HD23	1:B:83:ILE:HG23	2.02	0.41
1:B:149:TYR:HB2	1:B:204:HIS:CD2	2.54	0.41
2:K:49:ASP:O	2:K:50:ASN:HB2	2.20	0.41
2:K:126:GLU:HG2	2:K:131:LYS:O	2.19	0.41
2:L:78:GLN:OE1	2:L:78:GLN:HA	2.21	0.41
2:C:183:THR:HG22	2:C:184:PRO:HD2	2.02	0.41
3:O:55:LEU:HD21	3:O:57:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:68:PHE:N	1:J:68:PHE:CD1	2.88	0.41
1:J:166:GLY:O	1:J:186:VAL:HA	2.20	0.41
3:T:81:MET:HE2	3:T:81:MET:HB3	1.98	0.41
2:E:82:GLU:HG3	2:E:105:LEU:O	2.20	0.41
3:O:81:MET:O	3:O:84:ARG:O	2.38	0.41
1:J:169:THR:HG23	1:J:184:SER:HB3	2.02	0.41
2:K:183:THR:OG1	2:K:186:GLN:HG3	2.21	0.41
3:N:61:SER:HB3	3:N:117:THR:HG23	2.03	0.41
1:B:33:ALA:C	1:B:34:MET:HG2	2.46	0.41
1:B:67:ARG:NH2	1:B:90:ASP:OD2	2.54	0.41
2:E:142:TYR:HB3	2:E:143:PRO:HD3	2.02	0.41
1:A:150:PHE:CD1	1:A:150:PHE:C	2.98	0.41
3:M:73:LEU:HA	3:M:76:MET:HE3	2.03	0.41
3:T:60:PRO:HA	3:T:116:THR:HG22	2.03	0.41
1:B:105:ASP:OD1	1:B:105:ASP:N	2.48	0.41
3:O:66:ARG:N	3:O:67:PRO:HD3	2.36	0.41
1:A:59:TYR:CG	3:T:24:LEU:HD12	2.56	0.41
1:B:34:MET:HA	1:B:99:LEU:HD12	2.02	0.41
1:D:83:ILE:HD12	1:D:86:LEU:HD21	2.02	0.40
1:D:197:THR:HG23	1:D:214:LYS:HE3	2.04	0.40
2:E:20:ILE:CG2	2:E:103:THR:HG21	2.51	0.40
3:M:35:ASN:O	3:M:38:GLN:HG2	2.21	0.40
2:K:35:TYR:CE2	2:K:88:GLN:HG2	2.56	0.40
1:D:68:PHE:CD1	1:D:68:PHE:N	2.88	0.40
2:E:31:ASP:HB3	2:E:50:ASN:OD1	2.21	0.40
2:E:138:ILE:HG12	2:E:197:VAL:HG21	2.04	0.40
2:E:143:PRO:HD2	2:E:199:HIS:CE1	2.56	0.40
2:L:60:ARG:HB2	2:L:75:SER:O	2.22	0.40
3:O:33:LEU:O	3:O:37:MET:HG2	2.21	0.40
3:T:87:LEU:HG	3:T:91:ARG:NH2	2.37	0.40
1:J:37:VAL:HG21	1:J:107:TRP:CH2	2.57	0.40
1:B:59:TYR:CG	3:O:24:LEU:HD13	2.56	0.40
1:D:53:ASN:ND2	1:D:53:ASN:O	2.55	0.40
2:E:26:SER:HB2	2:E:90:TYR:O	2.21	0.40
2:K:27:LEU:HA	2:K:30:TYR:O	2.22	0.40
2:K:142:TYR:CD1	2:K:142:TYR:C	2.99	0.40

All (4) 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:C:158:LYS:O	2:K:23:GLN:NE2[1_465]	2.10	0.10
2:L:128:GLN:NE2	1:B:119:SER:O[1_546]	2.11	0.09
1:D:207:SER:O	1:J:213:LYS:NZ[1_564]	2.13	0.07
2:L:128:GLN:HE22	1:B:119:SER:O[1_546]	1.55	0.05

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	208/220 (94%)	200 (96%)	6 (3%)	2 (1%)	12	41
1	B	209/220 (95%)	200 (96%)	8 (4%)	1 (0%)	24	55
1	D	206/220 (94%)	197 (96%)	8 (4%)	1 (0%)	24	55
1	J	204/220 (93%)	197 (97%)	6 (3%)	1 (0%)	24	55
2	C	208/214 (97%)	191 (92%)	17 (8%)	0	100	100
2	E	207/214 (97%)	197 (95%)	10 (5%)	0	100	100
2	K	207/214 (97%)	196 (95%)	11 (5%)	0	100	100
2	L	207/214 (97%)	197 (95%)	10 (5%)	0	100	100
3	M	118/130 (91%)	112 (95%)	6 (5%)	0	100	100
3	N	117/130 (90%)	112 (96%)	4 (3%)	1 (1%)	14	43
3	O	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
3	T	113/130 (87%)	107 (95%)	3 (3%)	3 (3%)	4	22
All	All	2109/2256 (94%)	2009 (95%)	91 (4%)	9 (0%)	30	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASP
3	T	64	CYS
3	T	65	THR
1	J	194	GLY

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Mol	Chain	Res	Type
3	N	62	ASP
3	T	61	SER
1	B	153	PRO
1	D	152	GLU
1	A	153	PRO

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	177/184 (96%)	177 (100%)	0	100	100
1	B	178/184 (97%)	178 (100%)	0	100	100
1	D	176/184 (96%)	176 (100%)	0	100	100
1	J	176/184 (96%)	174 (99%)	2 (1%)	65	75
2	C	175/179 (98%)	175 (100%)	0	100	100
2	E	174/179 (97%)	174 (100%)	0	100	100
2	K	174/179 (97%)	174 (100%)	0	100	100
2	L	174/179 (97%)	174 (100%)	0	100	100
3	M	110/118 (93%)	110 (100%)	0	100	100
3	N	110/118 (93%)	110 (100%)	0	100	100
3	O	103/118 (87%)	103 (100%)	0	100	100
3	T	109/118 (92%)	109 (100%)	0	100	100
All	All	1836/1924 (95%)	1834 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	192	SER
1	J	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
3	T	75	GLN
1	B	175	GLN
3	O	111	GLN
2	E	196	GLN
3	M	31	ASN
3	M	35	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
4	SO4	B	301	-	4,4,4	0.25	0	6,6,6	0.22	0
4	SO4	M	202	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	A	301	-	4,4,4	0.24	0	6,6,6	0.11	0
4	SO4	M	201	-	4,4,4	0.23	0	6,6,6	0.12	0
4	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.27	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	SO4	1	0
4	M	202	SO4	1	0
4	M	201	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	212/220 (96%)	-0.33	0 100 100	49, 74, 107, 123	0
1	B	213/220 (96%)	-0.25	0 100 100	49, 83, 113, 130	0
1	D	210/220 (95%)	-0.18	0 100 100	61, 91, 115, 123	0
1	J	210/220 (95%)	-0.17	0 100 100	54, 85, 122, 154	0
2	C	210/214 (98%)	-0.04	0 100 100	56, 93, 120, 126	0
2	E	209/214 (97%)	-0.15	1 (0%) 87 77	61, 89, 108, 126	0
2	K	209/214 (97%)	-0.28	0 100 100	56, 84, 108, 126	0
2	L	209/214 (97%)	-0.33	1 (0%) 87 77	48, 76, 104, 121	0
3	M	120/130 (92%)	0.04	2 (1%) 69 51	57, 85, 117, 145	0
3	N	119/130 (91%)	0.11	2 (1%) 69 51	55, 82, 119, 139	0
3	O	111/130 (85%)	0.01	1 (0%) 81 67	69, 95, 117, 145	0
3	T	117/130 (90%)	-0.06	0 100 100	54, 85, 127, 141	0
All	All	2149/2256 (95%)	-0.16	7 (0%) 90 83	48, 85, 115, 154	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	144	GLY	3.9
3	N	85	TYR	2.8
3	M	110	GLU	2.2
3	N	48	SER	2.1
3	M	109	CYS	2.1
3	O	65	THR	2.1
2	E	3	ALA	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	SO4	B	301	5/5	0.76	0.08	82,82,93,143	0
4	SO4	A	301	5/5	0.83	0.09	62,70,81,107	0
4	SO4	D	301	5/5	0.83	0.08	86,88,102,139	0
4	SO4	M	201	5/5	0.83	0.07	90,93,106,122	0
4	SO4	M	202	5/5	0.88	0.09	80,91,104,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.