Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:07 PM GMT

PDB ID	:	4XCY
Title	:	Crystal structure of human 4E10 Fab in complex with phosphatidylglycerol (06:0 PG)
Authors	:	Irimia, A.; Stanfield, R.L.; Wilson, I.A.
Deposited on	:	2014-12-18
Resolution	:	3.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

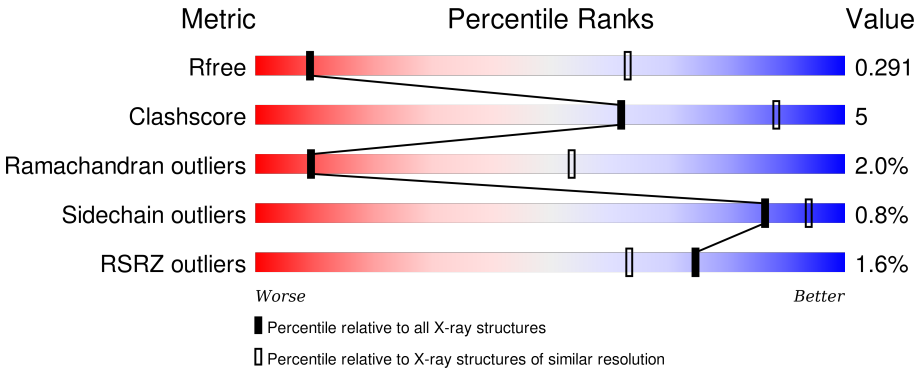
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1011 (4.38-3.54)
Clashscore	102246	1025 (4.32-3.60)
Ramachandran outliers	100387	1008 (4.34-3.58)
Sidechain outliers	100360	1027 (4.36-3.56)
RSRZ outliers	91569	1015 (4.38-3.54)

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 <=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	B	215	2% 79% 21%
1	D	215	86% 11%
1	F	215	81% 18%
1	I	215	% 86% 11%
1	K	215	3% 87% 11%

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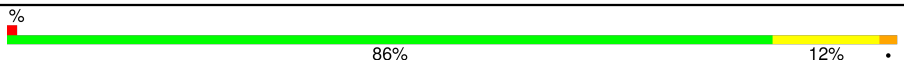
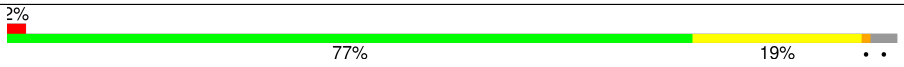
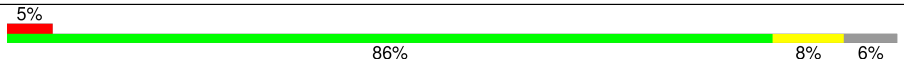
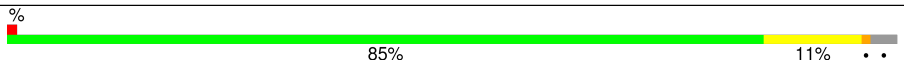
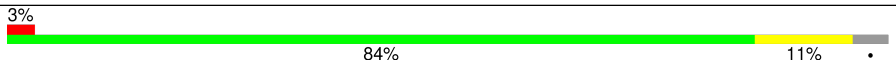
Mol	Chain	Length	Quality of chain
1	L	215	
2	A	230	
2	C	230	
2	E	230	
2	G	230	
2	H	230	
2	J	230	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNL	F	301	-	-	-	X
3	UNL	K	301	-	-	-	X
4	44G	A	301	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19410 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 4E10 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	1	0
			1618	1005	280	328	5			
1	B	214	Total	C	N	O	S	0	1	0
			1625	1007	280	333	5			
1	D	214	Total	C	N	O	S	0	0	0
			1605	994	276	331	4			
1	F	214	Total	C	N	O	S	0	1	0
			1588	986	275	322	5			
1	I	211	Total	C	N	O	S	0	0	0
			1567	971	269	323	4			
1	K	212	Total	C	N	O	S	0	1	0
			1582	977	274	326	5			

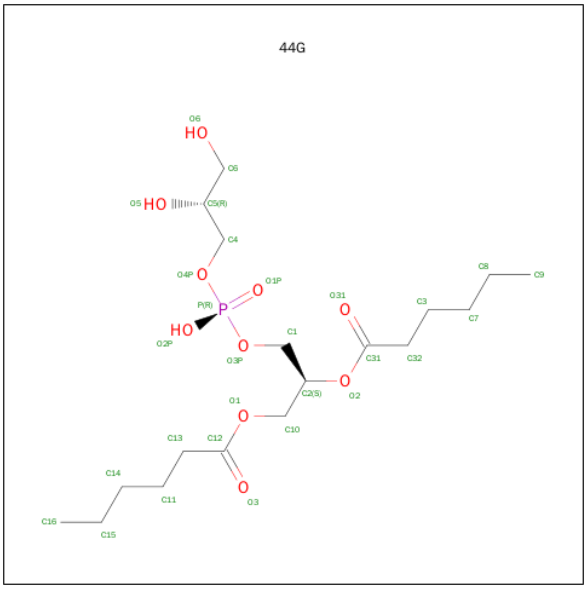
- Molecule 2 is a protein called 4E10 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	3	0
			1661	1055	280	318	8			
2	A	228	Total	C	N	O	S	0	4	0
			1668	1057	280	323	8			
2	C	221	Total	C	N	O	S	0	3	0
			1607	1014	270	315	8			
2	E	223	Total	C	N	O	S	0	1	0
			1611	1017	272	316	6			
2	G	216	Total	C	N	O	S	0	2	0
			1538	971	255	305	7			
2	J	221	Total	C	N	O	S	0	2	0
			1592	1007	265	313	7			

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

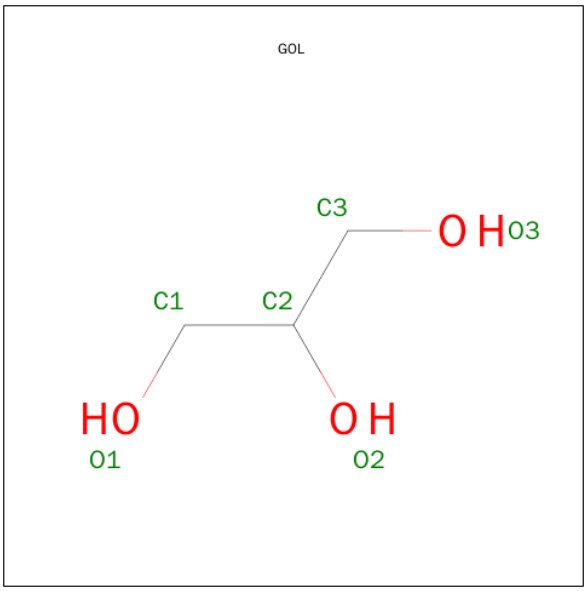
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 21 14 7	0	0
3	B	1	Total C O 21 14 7	0	0
3	L	1	Total C O 21 14 7	0	0
3	K	1	Total C O 21 14 7	0	0
3	F	1	Total C O 21 14 7	0	0

- Molecule 4 is (2S)-3-{[(R)-{[(2R)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-2-(hexanoyloxy)propyl hexanoate (three-letter code: 44G) (formula: $C_{18}H_{35}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O P 16 7 8 1	0	0
4	A	1	Total C O P 21 10 10 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



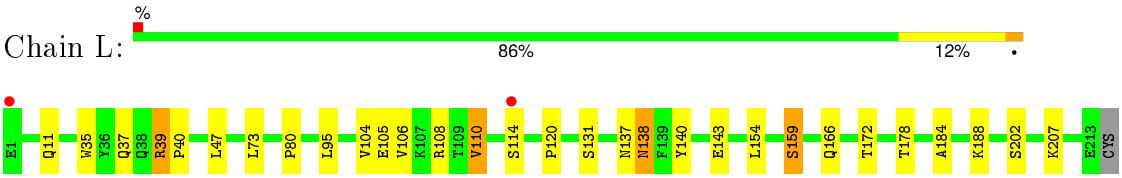
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

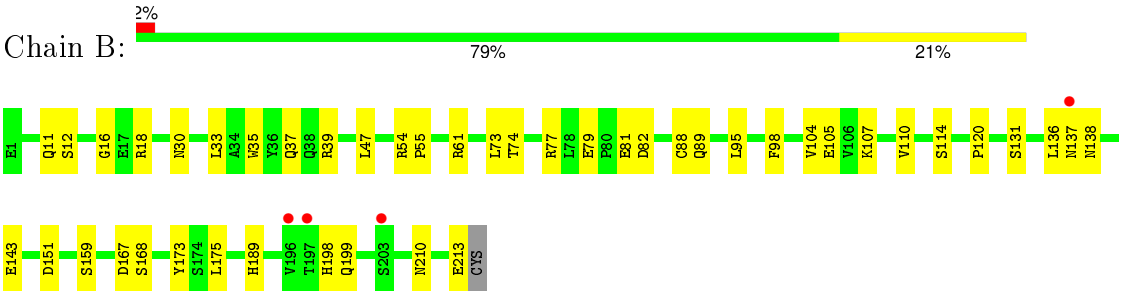
- Molecule 1: 4E10 Fab light chain

Chain L:



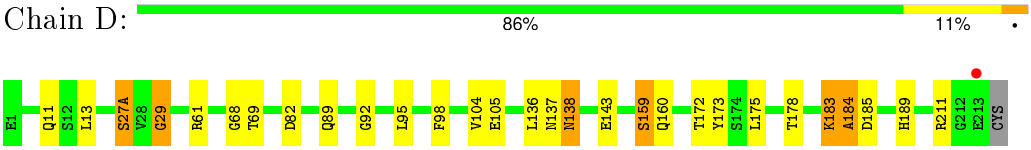
- Molecule 1: 4E10 Fab light chain

Chain B:



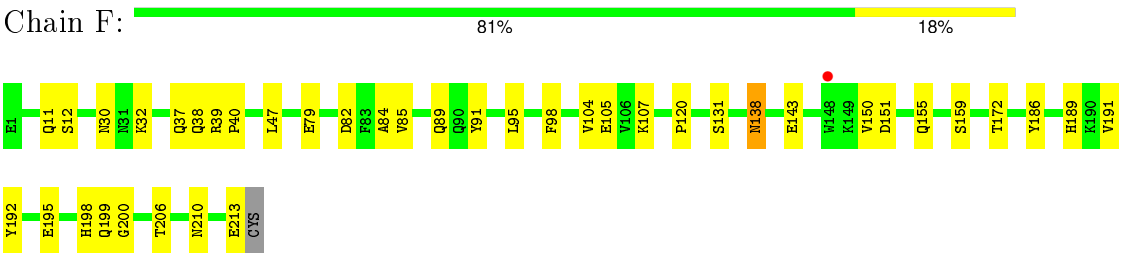
- Molecule 1: 4E10 Fab light chain

Chain D:



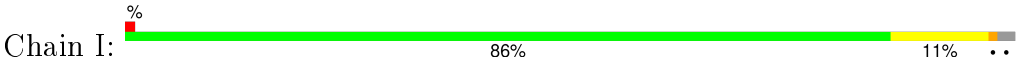
- Molecule 1: 4E10 Fab light chain

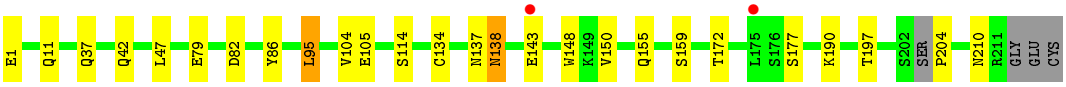
Chain F:



- Molecule 1: 4E10 Fab light chain

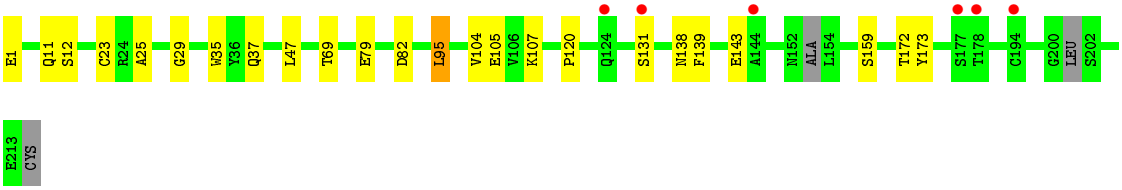
Chain I:





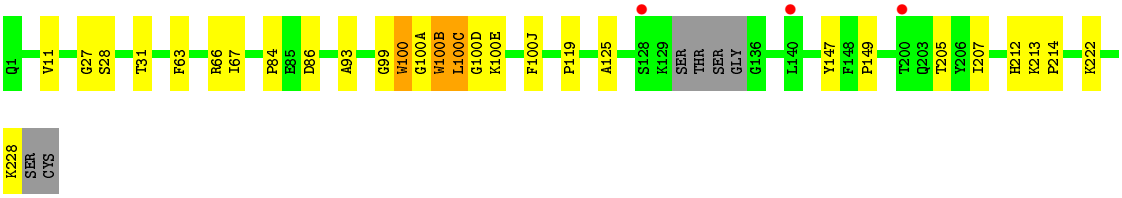
• Molecule 1: 4E10 Fab light chain

Chain K:



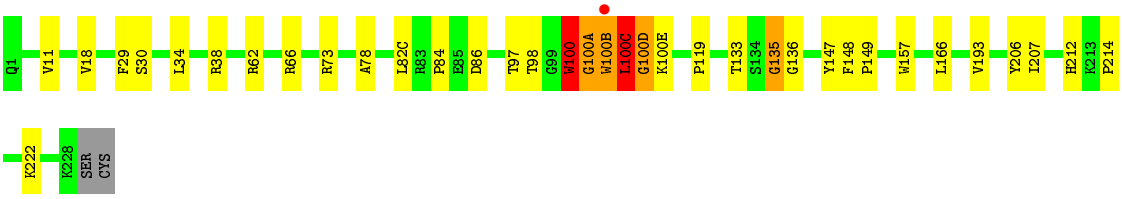
• Molecule 2: 4E10 Fab heavy chain

Chain H:



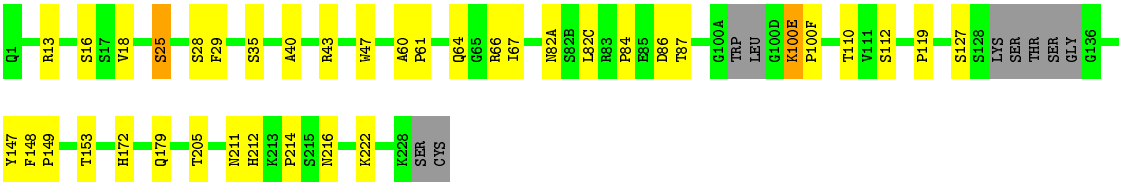
• Molecule 2: 4E10 Fab heavy chain

Chain A:



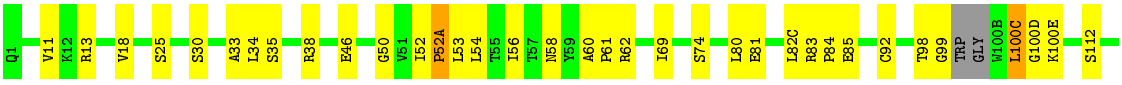
• Molecule 2: 4E10 Fab heavy chain

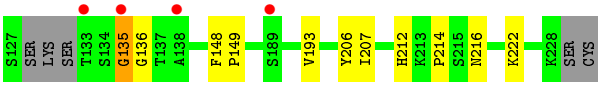
Chain C:



• Molecule 2: 4E10 Fab heavy chain

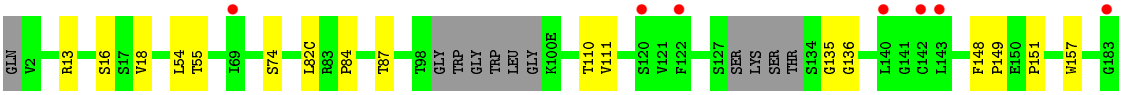
Chain E:

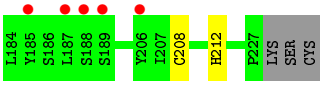




• Molecule 2: 4E10 Fab heavy chain

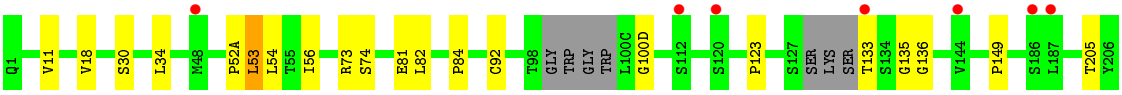
Chain G:





• Molecule 2: 4E10 Fab heavy chain

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	150.22Å 150.22Å 472.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.91 – 3.96 48.91 – 3.96	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.91-3.96) 95.6 (48.91-3.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.30	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.244 , 0.291 0.250 , 0.291	Depositor DCC
R_{free} test set	1362 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	62.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 27266 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	19410	wwPDB-VP
Average B, all atoms (Å^2)	77.0	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 36.35 % 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 5.0693e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UNL, GOL, 44G

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	B	0.24	0/1661	0.49	0/2258
1	D	0.28	0/1638	0.56	0/2230
1	F	0.28	0/1624	0.56	0/2213
1	I	0.25	0/1599	0.49	0/2179
1	K	0.24	0/1616	0.49	0/2199
1	L	0.33	0/1654	0.65	3/2247 (0.1%)
2	A	0.24	0/1723	0.51	1/2362 (0.0%)
2	C	0.25	0/1653	0.52	0/2262
2	E	0.27	0/1651	0.56	1/2261 (0.0%)
2	G	0.24	0/1581	0.48	0/2173
2	H	0.24	0/1712	0.51	0/2340
2	J	0.24	0/1635	0.50	1/2242 (0.0%)
All	All	0.26	0/19747	0.53	6/26966 (0.0%)

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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	39	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	L	39	ARG	NH1-CZ-NH2	7.12	127.23	119.40
2	A	100(A)	GLY	N-CA-C	-7.01	95.56	113.10
1	L	39	ARG	NE-CZ-NH1	-6.07	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	100(E)	LYS	N-CA-C	-5.45	96.29	111.00
2	J	53	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	29	GLY	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	B	1625	0	1549	22	0
1	D	1605	0	1510	19	0
1	F	1588	0	1492	20	0
1	I	1567	0	1447	13	0
1	K	1582	0	1466	11	0
1	L	1618	0	1545	14	0
2	A	1668	0	1621	23	0
2	C	1607	0	1559	22	0
2	E	1611	0	1557	26	0
2	G	1538	0	1451	11	0
2	H	1661	0	1642	20	0
2	J	1592	0	1536	15	0
3	B	21	0	0	0	0
3	D	21	0	0	0	0
3	F	21	0	0	1	0
3	K	21	0	0	0	0
3	L	21	0	0	0	0
4	A	21	0	13	4	0
4	H	16	0	10	4	0
5	A	6	0	8	0	0
All	All	19410	0	18406	204	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 5.

All (204) 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:D:183:LYS:HG2	1:D:184:ALA:H	1.38	0.87
2:E:98:THR:H	2:E:100(D):GLY:HA2	1.40	0.86
2:E:52(A):PRO:O	2:E:54:LEU:N	2.16	0.78
1:B:11:GLN:HB3	1:B:104:VAL:HA	1.68	0.76
2:H:100(B):TRP:HE1	4:H:301:44G:H6	1.51	0.75
2:C:66:ARG:NH1	2:C:86:ASP:OD1	2.21	0.71
2:H:100(E):LYS:HD2	2:G:74:SER:HA	1.73	0.70
1:F:12:SER:HB3	1:F:107:LYS:HD3	1.77	0.67
1:L:39:ARG:HB3	1:L:40:PRO:HD2	1.78	0.66
1:L:39:ARG:HB3	1:L:40:PRO:CD	2.26	0.65
2:A:100(C):LEU:HD12	2:A:100(D):GLY:H	1.61	0.65
1:F:11:GLN:HB3	1:F:104:VAL:HA	1.80	0.64
1:D:27(A):SER:H	1:D:69:THR:HG22	1.64	0.63
2:A:73:ARG:NH1	4:A:301:44G:O5	2.32	0.63
2:H:205:THR:HG23	2:H:222:LYS:HE3	1.82	0.62
1:B:120:PRO:HB3	1:B:131:SER:H	1.66	0.61
1:D:183:LYS:O	1:D:185:ASP:N	2.31	0.61
2:J:30:SER:O	2:J:52(A):PRO:HG2	2.03	0.59
2:J:54:LEU:HB2	2:J:56:ILE:HG12	1.84	0.59
1:D:138:ASN:ND2	1:D:172:THR:OG1	2.32	0.59
1:D:136:LEU:HB2	1:D:175:LEU:HB3	1.85	0.59
2:C:25:SER:OG	2:E:74:SER:O	2.21	0.59
2:A:38:ARG:NH1	2:A:62:ARG:HH12	2.01	0.58
2:A:66:ARG:NH1	2:A:86:ASP:OD1	2.32	0.58
2:C:28:SER:OG	2:C:29:PHE:N	2.37	0.57
1:L:11:GLN:HB3	1:L:104:VAL:HA	1.85	0.57
1:I:197:THR:HG22	1:I:204:PRO:HG3	1.86	0.57
2:C:205:THR:HG23	2:C:222:LYS:HE3	1.86	0.56
1:K:11:GLN:HB3	1:K:104:VAL:HA	1.86	0.55
2:A:97:THR:HG21	2:A:100:TRP:CD1	2.41	0.55
1:I:114:SER:HB2	1:I:137:ASN:HB3	1.87	0.55
2:J:11:VAL:HG21	2:J:149:PRO:HG3	1.87	0.55
2:A:100(A):GLY:O	2:A:100(C):LEU:N	2.40	0.54
1:I:150:VAL:HB	1:I:155:GLN:NE2	2.23	0.54
1:L:202:SER:HB3	1:B:110:VAL:HG12	1.90	0.54
2:E:33:ALA:HB2	2:E:52:ILE:HG12	1.90	0.54
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.89	0.54
1:F:79:GLU:O	1:F:82:ASP:N	2.39	0.53
1:F:120:PRO:HB3	1:F:131:SER:H	1.73	0.53
1:D:11:GLN:HB3	1:D:104:VAL:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:GLU:OE1	1:K:29:GLY:HA3	2.08	0.53
2:E:11:VAL:HG21	2:E:149:PRO:HG3	1.91	0.53
2:E:38:ARG:HH11	2:E:62:ARG:HH12	1.56	0.53
1:D:29:GLY:O	1:D:92:GLY:HA3	2.09	0.53
2:G:87:THR:HG23	2:G:110:THR:HA	1.90	0.53
1:B:105:GLU:OE2	1:B:173:TYR:OH	2.21	0.53
2:H:27:GLY:HA2	2:H:100:TRP:NE1	2.24	0.53
1:D:160:GLN:HE22	2:C:179:GLN:HA	1.73	0.52
2:E:30:SER:O	2:E:52(A):PRO:HG2	2.08	0.52
1:B:151:ASP:OD2	1:B:189:HIS:ND1	2.34	0.52
1:F:11:GLN:O	1:F:105:GLU:HG2	2.10	0.52
2:E:99:GLY:HA3	2:E:100(C):LEU:HB2	1.92	0.51
1:I:134:CYS:HB2	1:I:148:TRP:CH2	2.45	0.51
2:A:11:VAL:HG21	2:A:149:PRO:HG3	1.93	0.51
1:I:148:TRP:HZ2	1:I:177:SER:HG	1.58	0.51
1:I:79:GLU:O	1:I:82:ASP:N	2.42	0.51
1:D:183:LYS:HG2	1:D:184:ALA:N	2.16	0.51
2:A:100(B):TRP:O	2:J:53:LEU:HD11	2.11	0.51
1:K:120:PRO:HB3	1:K:131:SER:H	1.76	0.51
1:B:61:ARG:NE	1:B:82:ASP:OD2	2.44	0.50
2:J:205:THR:HG23	2:J:222:LYS:HE3	1.92	0.50
2:H:93:ALA:HB1	2:H:100(J):PHE:HB3	1.93	0.50
2:G:18:VAL:HB	2:G:82(C):LEU:HD11	1.94	0.50
2:A:100(B):TRP:HE1	4:A:301:44G:H16	1.76	0.50
2:H:63:PHE:O	2:H:67:ILE:HG22	2.12	0.50
1:I:1:GLU:HG3	1:I:95:LEU:HD21	1.93	0.50
1:I:11:GLN:O	1:I:105:GLU:HG2	2.12	0.50
2:A:212:HIS:CD2	2:A:214:PRO:HD2	2.47	0.49
1:B:16:GLY:HA2	1:B:77:ARG:HG3	1.95	0.49
2:C:87:THR:HG23	2:C:110:THR:HA	1.93	0.49
2:J:212:HIS:CD2	2:J:214:PRO:HD2	2.48	0.49
1:D:159:SER:HA	1:D:178:THR:O	2.13	0.49
1:D:27(A):SER:HA	1:D:68:GLY:O	2.13	0.48
1:L:120:PRO:HB3	1:L:131:SER:H	1.78	0.48
2:A:100(E):LYS:HE3	2:J:74:SER:HA	1.95	0.48
2:A:119:PRO:HB3	2:A:147:TYR:HB3	1.94	0.48
2:C:66:ARG:HB2	2:C:82(A):ASN:O	2.13	0.48
2:A:29:PHE:N	4:A:301:44G:O2P	2.47	0.48
2:J:53:LEU:HA	2:J:73:ARG:HD2	1.94	0.48
2:C:18:VAL:HB	2:C:82(C):LEU:HD11	1.95	0.48
1:F:150:VAL:HB	1:F:155:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:ASN:ND2	1:F:172:THR:OG1	2.41	0.48
1:I:82:ASP:O	1:I:86:TYR:OH	2.24	0.48
2:A:207:ILE:HG22	2:A:222:LYS:HA	1.95	0.47
2:H:100(A):GLY:O	2:H:100(C):LEU:N	2.47	0.47
2:E:34:LEU:HD21	2:E:92[B]:CYS:SG	2.54	0.47
2:C:35:SER:HB3	2:C:47:TRP:HE1	1.79	0.47
1:K:23:CYS:HB2	1:K:35:TRP:CH2	2.50	0.47
1:B:11:GLN:O	1:B:105:GLU:HG2	2.15	0.47
1:L:35:TRP:CD2	1:L:73:LEU:HB2	2.50	0.47
1:I:190:LYS:O	1:I:210:ASN:HA	2.16	0.46
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.97	0.46
2:E:18:VAL:HB	2:E:82(C):LEU:HD11	1.97	0.46
1:L:106:VAL:O	1:L:166:GLN:NE2	2.47	0.46
1:F:186:TYR:HA	1:F:192:TYR:OH	2.15	0.46
1:L:184:ALA:O	1:L:188:LYS:HG3	2.16	0.46
2:C:64:GLN:HA	2:C:67:ILE:HG22	1.97	0.46
2:E:193:VAL:HG11	2:E:206:TYR:CE1	2.50	0.46
2:H:11:VAL:HG21	2:H:149:PRO:HG3	1.98	0.46
2:H:100(B):TRP:NE1	4:H:301:44G:H6	2.25	0.45
2:J:207:ILE:HG22	2:J:222:LYS:HA	1.98	0.45
2:A:100(C):LEU:CD1	2:A:100(D):GLY:H	2.29	0.45
1:I:11:GLN:HB3	1:I:104:VAL:HA	1.98	0.45
1:F:38:GLN:O	1:F:84:ALA:HB1	2.16	0.45
1:B:210:ASN:HB2	1:B:213:GLU:HB3	1.99	0.45
2:H:31:THR:HG21	2:H:100(B):TRP:HA	1.97	0.45
1:F:195:GLU:HA	1:F:206:THR:HG22	1.99	0.45
2:E:98:THR:N	2:E:100(D):GLY:HA2	2.21	0.45
2:H:31:THR:OG1	2:G:54:LEU:HD21	2.16	0.45
2:C:13:ARG:O	2:C:16:SER:OG	2.29	0.45
1:B:12:SER:HB3	1:B:107:LYS:HD3	1.98	0.45
1:K:12:SER:HB3	1:K:107:LYS:HB2	1.99	0.45
1:B:54:ARG:HA	1:B:55:PRO:HD3	1.87	0.45
1:K:105:GLU:OE2	1:K:173:TYR:OH	2.27	0.45
1:D:105:GLU:OE2	1:D:173:TYR:OH	2.23	0.45
2:J:123:PRO:HD3	2:J:221:LYS:HE2	1.99	0.45
1:B:114:SER:HB2	1:B:137:ASN:HB3	1.99	0.45
1:F:32:LYS:HD2	1:F:91:TYR:CE2	2.52	0.45
2:J:18:VAL:O	2:J:81:GLU:HA	2.16	0.44
2:C:100(E):LYS:HA	2:C:100(F):PRO:HD2	1.85	0.44
2:C:119:PRO:HB3	2:C:147:TYR:HB3	1.99	0.44
1:B:89:GLN:HB2	1:B:98:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:97:THR:OG1	2:A:98:THR:N	2.51	0.44
1:D:11:GLN:O	1:D:105:GLU:HG2	2.18	0.44
2:H:207:ILE:HG22	2:H:222:LYS:HA	1.99	0.44
2:G:135:GLY:HA3	2:G:136:GLY:HA3	1.71	0.44
2:E:35:SER:HA	2:E:50:GLY:HA2	1.99	0.44
2:C:13:ARG:HG2	2:E:216:ASN:OD1	2.17	0.44
1:L:114:SER:HB2	1:L:137:ASN:HB3	1.98	0.44
1:K:1:GLU:HG3	1:K:95:LEU:HD21	2.00	0.44
1:F:89:GLN:HB2	1:F:98:PHE:CD1	2.53	0.44
2:C:212:HIS:CD2	2:C:214:PRO:HD2	2.53	0.43
2:C:216:ASN:OD1	2:E:13:ARG:HG3	2.18	0.43
2:A:148:PHE:HA	2:A:149:PRO:HA	1.74	0.43
2:H:28:SER:HB2	4:H:301:44G:H5	2.00	0.43
2:H:212:HIS:CD2	2:H:214:PRO:HD2	2.53	0.43
2:C:112:SER:HB3	2:C:148:PHE:CZ	2.52	0.43
2:G:148:PHE:HA	2:G:149:PRO:HA	1.77	0.43
2:H:28:SER:CB	4:H:301:44G:H5	2.49	0.43
1:L:159:SER:HA	1:L:178:THR:O	2.18	0.43
2:A:18:VAL:HB	2:A:82(C):LEU:HD11	2.01	0.43
1:F:151:ASP:OD2	1:F:189:HIS:ND1	2.34	0.43
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.99	0.43
1:L:110:VAL:HG23	1:L:140:TYR:O	2.17	0.43
1:B:79:GLU:O	1:B:82:ASP:N	2.48	0.43
2:C:40:ALA:HB3	2:C:43:ARG:HB2	2.01	0.43
1:F:198:HIS:CG	1:F:199:GLN:N	2.87	0.43
2:E:46:GLU:OE2	2:E:62:ARG:NH1	2.52	0.43
2:E:112:SER:HB3	2:E:148:PHE:CZ	2.54	0.42
2:E:148:PHE:HA	2:E:149:PRO:HA	1.69	0.42
2:E:83:ARG:NH1	2:E:85:GLU:OE2	2.52	0.42
1:K:25:ALA:HB3	1:K:69:THR:HA	2.02	0.42
2:H:149:PRO:HD2	2:H:214:PRO:HB2	2.00	0.42
2:G:55:THR:O	2:G:55:THR:HG22	2.20	0.42
2:G:82(C):LEU:HD13	2:G:111:VAL:HG22	2.01	0.42
1:D:61:ARG:NE	1:D:82:ASP:OD2	2.51	0.42
1:F:85:VAL:HG21	3:F:301:UNL:C6	2.49	0.42
1:D:11:GLN:HG3	1:D:13:LEU:HG	2.01	0.42
2:G:157:TRP:CH2	2:G:208:CYS:HB3	2.55	0.42
1:D:136:LEU:HD13	1:D:175:LEU:HD22	2.02	0.41
2:E:207:ILE:HG22	2:E:222:LYS:HA	2.00	0.41
1:B:35:TRP:CD2	1:B:73:LEU:HB2	2.55	0.41
2:A:193:VAL:HG11	2:A:206:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:ILE:HG12	2:E:80:LEU:HD13	2.02	0.41
1:B:18:ARG:NH1	1:B:74:THR:HG21	2.35	0.41
1:K:37:GLN:HB2	1:K:47:LEU:HD11	2.02	0.41
1:F:39:ARG:HB3	1:F:40:PRO:CD	2.50	0.41
1:B:167:ASP:OD1	1:B:168:SER:N	2.54	0.41
1:B:39:ARG:HH21	1:B:81:GLU:HB3	1.85	0.41
2:H:213:LYS:HB2	2:H:214:PRO:HD3	2.02	0.41
2:C:148:PHE:HA	2:C:149:PRO:HA	1.84	0.41
2:A:34:LEU:HD13	2:A:78:ALA:HB2	2.02	0.41
2:J:34:LEU:HD11	2:J:92[B]:CYS:SG	2.61	0.41
2:J:82:LEU:HD12	2:J:82:LEU:HA	1.94	0.41
2:C:60:ALA:HA	2:C:61:PRO:HD3	1.92	0.41
1:L:138:ASN:ND2	1:L:172:THR:OG1	2.51	0.41
2:J:135:GLY:HA3	2:J:136:GLY:HA3	1.81	0.41
1:I:138:ASN:ND2	1:I:172:THR:OG1	2.52	0.41
2:G:151:PRO:O	2:G:212:HIS:HD2	2.03	0.41
2:G:13:ARG:O	2:G:16:SER:OG	2.27	0.41
1:L:11:GLN:O	1:L:105:GLU:HG2	2.21	0.41
1:I:37:GLN:HB2	1:I:47:LEU:HD11	2.03	0.41
2:E:60:ALA:HA	2:E:61:PRO:HD3	1.90	0.41
1:B:136:LEU:HB2	1:B:175:LEU:HB3	2.03	0.41
2:H:66:ARG:NH1	2:H:86:ASP:OD1	2.53	0.41
2:H:119:PRO:HB3	2:H:147:TYR:HB3	2.03	0.41
1:F:151:ASP:HA	1:F:191:VAL:HB	2.03	0.40
1:K:79:GLU:O	1:K:82:ASP:N	2.47	0.40
2:C:153:THR:OG1	2:C:211:ASN:HB3	2.21	0.40
2:E:56:ILE:HD11	2:J:54:LEU:HD12	2.03	0.40
2:E:135:GLY:N	2:E:136:GLY:O	2.55	0.40
2:H:125:ALA:HB3	2:H:228:LYS:HE3	2.03	0.40
2:A:157:TRP:HB3	2:A:166:LEU:HD23	2.03	0.40
2:A:30:SER:OG	4:A:301:44G:H8	2.21	0.40
1:D:89:GLN:HB2	1:D:98:PHE:CD1	2.57	0.40
1:B:198:HIS:CG	1:B:199:GLN:N	2.89	0.40
1:F:198:HIS:CE1	1:F:200:GLY:H	2.39	0.40
1:F:210:ASN:HB2	1:F:213:GLU:CB	2.52	0.40
1:K:139:PHE:N	1:K:172:THR:HB	2.37	0.40
1:D:137:ASN:HD21	2:C:172:HIS:CE1	2.39	0.40
2:E:212:HIS:CD2	2:E:214:PRO:HD2	2.56	0.40
1:B:33:LEU:HD11	1:B:88:CYS:HB2	2.04	0.40
1:D:189:HIS:O	1:D:211:ARG:NE	2.44	0.40
2:A:135:GLY:N	2:A:136:GLY:O	2.55	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	B	213/215 (99%)	198 (93%)	12 (6%)	3 (1%)	14 59
1	D	212/215 (99%)	195 (92%)	11 (5%)	6 (3%)	6 46
1	F	213/215 (99%)	196 (92%)	14 (7%)	3 (1%)	14 59
1	I	207/215 (96%)	192 (93%)	12 (6%)	3 (1%)	14 59
1	K	207/215 (96%)	192 (93%)	12 (6%)	3 (1%)	14 59
1	L	213/215 (99%)	196 (92%)	11 (5%)	6 (3%)	6 46
2	A	230/230 (100%)	205 (89%)	19 (8%)	6 (3%)	7 48
2	C	218/230 (95%)	200 (92%)	14 (6%)	4 (2%)	11 55
2	E	218/230 (95%)	197 (90%)	15 (7%)	6 (3%)	6 46
2	G	212/230 (92%)	195 (92%)	16 (8%)	1 (0%)	34 76
2	H	223/230 (97%)	201 (90%)	16 (7%)	6 (3%)	6 47
2	J	217/230 (94%)	198 (91%)	16 (7%)	3 (1%)	14 59
All	All	2583/2670 (97%)	2365 (92%)	168 (6%)	50 (2%)	9 54

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	110	VAL
2	C	127	SER
2	E	52(A)	PRO
2	E	53	LEU
1	L	143	GLU
2	H	100(B)	TRP
1	B	143	GLU
2	A	100(B)	TRP
2	A	135	GLY

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Mol	Chain	Res	Type
1	D	27(A)	SER
1	D	143	GLU
2	C	25	SER
1	F	143	GLU
2	E	135	GLY
1	I	143	GLU
1	K	143	GLU
2	J	227	PRO
1	L	159	SER
2	H	100	TRP
2	H	100(D)	GLY
1	B	159	SER
2	A	100	TRP
2	A	100(C)	LEU
2	A	100(D)	GLY
1	D	159	SER
1	D	183	LYS
1	D	184	ALA
2	C	100(E)	LYS
1	F	159	SER
2	E	25	SER
1	I	159	SER
1	K	159	SER
2	J	100(D)	GLY
1	L	138	ASN
2	H	100(C)	LEU
1	B	138	ASN
1	D	138	ASN
1	F	138	ASN
2	E	100(C)	LEU
1	I	138	ASN
1	K	138	ASN
1	L	154	LEU
2	H	99	GLY
2	J	84	PRO
1	L	80	PRO
2	H	84	PRO
2	A	84	PRO
2	C	84	PRO
2	E	84	PRO
2	G	84	PRO

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	B	181/185 (98%)	179 (99%)	2 (1%)	80 91
1	D	176/185 (95%)	175 (99%)	1 (1%)	90 95
1	F	172/185 (93%)	170 (99%)	2 (1%)	78 90
1	I	168/185 (91%)	166 (99%)	2 (1%)	78 90
1	K	172/185 (93%)	171 (99%)	1 (1%)	90 95
1	L	178/185 (96%)	175 (98%)	3 (2%)	68 88
2	A	182/189 (96%)	179 (98%)	3 (2%)	70 89
2	C	176/189 (93%)	176 (100%)	0	100 100
2	E	174/189 (92%)	173 (99%)	1 (1%)	90 95
2	G	165/189 (87%)	165 (100%)	0	100 100
2	H	184/189 (97%)	184 (100%)	0	100 100
2	J	173/189 (92%)	172 (99%)	1 (1%)	90 95
All	All	2101/2244 (94%)	2085 (99%)	16 (1%)	86 94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	95	LEU
1	L	108	ARG
1	L	207	LYS
1	B	30	ASN
1	B	95	LEU
2	A	100	TRP
2	A	100(C)	LEU
2	A	133	THR
1	D	95	LEU
1	F	30	ASN
1	F	95	LEU
2	E	58	ASN
1	I	42	GLN
1	I	95	LEU

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Mol	Chain	Res	Type
1	K	95	LEU
2	J	133	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	ASN
1	D	137	ASN
1	D	160	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 5 are unknown - leaving 3 for Mogul analysis.

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	44G	A	301	-	20,20,28	0.93	0	21,26,34	0.85	0
5	GOL	A	302	-	5,5,5	0.36	0	5,5,5	0.26	0
4	44G	H	301	-	15,15,28	0.79	0	16,19,34	0.63	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
4	44G	A	301	-	-	0/23/23/33	0/0/0/0
5	GOL	A	302	-	-	0/4/4/4	0/0/0/0
4	44G	H	301	-	-	0/16/16/33	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.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	44G	4	0
4	H	301	44G	4	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	B	214/215 (99%)	0.14	4 (1%)	70	59	24, 64, 106, 132	0
1	D	214/215 (99%)	0.02	1 (0%)	91	88	32, 75, 112, 224	0
1	F	214/215 (99%)	0.03	1 (0%)	91	88	33, 85, 130, 189	0
1	I	211/215 (98%)	0.17	2 (0%)	85	79	37, 88, 135, 179	0
1	K	212/215 (98%)	0.26	6 (2%)	56	44	34, 91, 141, 158	0
1	L	214/215 (99%)	0.12	2 (0%)	85	79	24, 66, 106, 158	0
2	A	228/230 (99%)	0.08	1 (0%)	93	90	16, 63, 116, 211	0
2	C	221/230 (96%)	0.03	0	100	100	19, 68, 113, 201	0
2	E	223/230 (96%)	0.10	4 (1%)	71	60	25, 64, 131, 184	0
2	G	216/230 (93%)	0.57	12 (5%)	28	20	34, 98, 145, 191	1 (0%)
2	H	224/230 (97%)	0.08	3 (1%)	79	70	21, 64, 104, 177	0
2	J	221/230 (96%)	0.45	7 (3%)	51	38	36, 83, 126, 160	0
All	All	2612/2670 (97%)	0.17	43 (1%)	74	63	16, 74, 130, 224	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	133	THR	3.4
2	G	189	SER	3.1
2	J	133	THR	3.0
2	G	188	SER	3.0
1	L	1	GLU	3.0
1	I	175	LEU	2.9
2	G	142[A]	CYS	2.8
1	B	196	VAL	2.6
2	G	185	TYR	2.6
2	H	140	LEU	2.5
2	G	187	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	148	TRP	2.5
1	K	178	THR	2.5
2	G	143	LEU	2.4
2	E	135	GLY	2.4
2	J	186	SER	2.3
2	G	122	PHE	2.3
1	B	197	THR	2.3
2	J	48	MET	2.3
2	E	189	SER	2.3
1	K	144	ALA	2.3
1	K	177	SER	2.3
2	G	120	SER	2.2
1	L	114	SER	2.2
1	B	203	SER	2.2
2	A	100(B)	TRP	2.2
2	E	138	ALA	2.2
2	J	120	SER	2.2
1	K	131	SER	2.1
2	G	183	GLY	2.1
2	J	144	VAL	2.1
2	G	69	ILE	2.1
1	I	143	GLU	2.1
2	J	112	SER	2.1
1	K	124	GLN	2.1
2	H	200	THR	2.1
2	G	206	TYR	2.1
1	K	194[A]	CYS	2.0
1	B	137	ASN	2.0
2	H	128	SER	2.0
2	J	187	LEU	2.0
2	G	140	LEU	2.0
1	D	213	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
3	UNL	F	301	21/-	0.71	0.43	2.76	105,105,105,105	0
3	UNL	D	301	21/-	0.77	0.36	1.43	98,98,98,98	0
4	44G	A	301	21/29	0.78	0.46	1.22	109,109,109,109	0
3	UNL	B	301	21/-	0.85	0.29	0.89	78,78,78,78	0
3	UNL	K	301	21/-	0.88	0.40	0.83	66,66,66,66	0
3	UNL	L	301	21/-	0.86	0.30	0.55	69,69,69,69	0
4	44G	H	301	16/29	0.90	0.26	-0.61	108,108,108,108	0
5	GOL	A	302	6/6	0.88	0.26	-	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.