



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:20 PM GMT

PDB ID : 4L8C  
Title : Crystal structure of the H2Db in complex with the NP-N3D peptide  
Authors : Rossjohn, J.; Gras, S.  
Deposited on : 2013-06-16  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

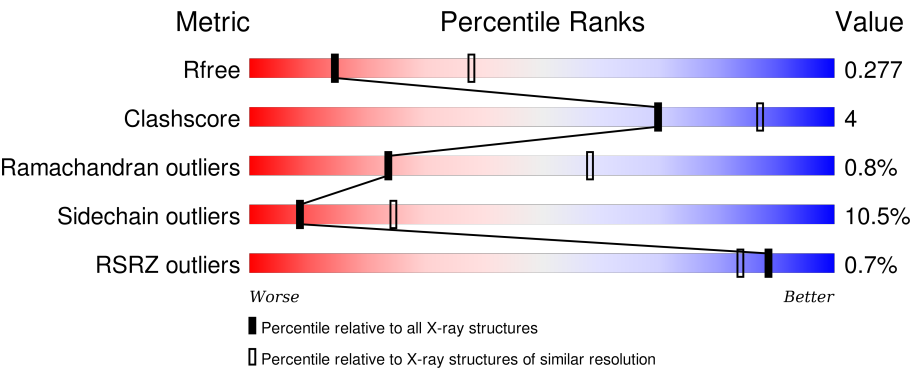
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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 <sub>free</sub>	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	<div><div></div><div>82%15%..</div></div>
1	C	280	<div><div>%</div><div>80%17%..</div></div>
1	E	280	<div><div>%</div><div>74%21%..</div></div>
1	G	280	<div><div>2%</div><div>79%15%...</div></div>
2	B	99	<div><div></div><div>84%14%. </div></div>

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Mol	Chain	Length	Quality of chain
2	D	99	<div><div></div><div>78%20%•</div></div>
2	F	99	<div><div></div><div>84%13%••</div></div>
2	H	99	<div><div></div><div>80%18%•</div></div>
3	I	9	<div><div></div><div>67%11%22%</div></div>
3	J	9	<div><div></div><div>78%22%</div></div>
3	K	9	<div><div></div><div>78%22%</div></div>
3	L	9	<div><div></div><div>67%22%11%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12637 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2257	1425	399	424	9			
1	C	275	Total	C	N	O	S	0	0	0
			2257	1425	399	424	9			
1	E	275	Total	C	N	O	S	0	0	0
			2257	1425	399	424	9			
1	G	275	Total	C	N	O	S	0	0	0
			2257	1425	399	424	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			801	512	135	147	7			
2	D	97	Total	C	N	O	S	0	0	0
			801	512	135	147	7			
2	F	98	Total	C	N	O	S	0	0	0
			810	517	137	149	7			
2	H	97	Total	C	N	O	S	0	0	0
			801	512	135	147	7			

- Molecule 3 is a protein called NP-N3D peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	S	0	0	0
			69	38	10	19	2			
3	J	9	Total	C	N	O	S	0	0	0
			69	38	10	19	2			
3	K	9	Total	C	N	O	S	0	0	0
			69	38	10	19	2			
3	L	9	Total	C	N	O	S	0	0	0
			69	38	10	19	2			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total	O	0	0
			15	15		
5	B	8	Total	O	0	0
			8	8		
5	C	15	Total	O	0	0
			15	15		
5	D	10	Total	O	0	0
			10	10		
5	E	19	Total	O	0	0
			19	19		
5	F	17	Total	O	0	0
			17	17		

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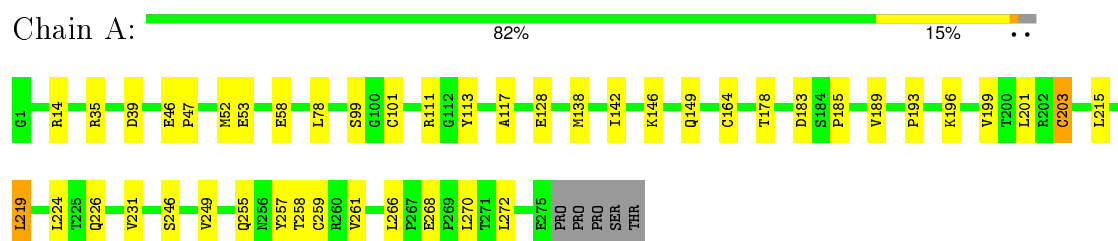
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	8	Total	O	0	0
			8	8		
5	H	3	Total	O	0	0
			3	3		

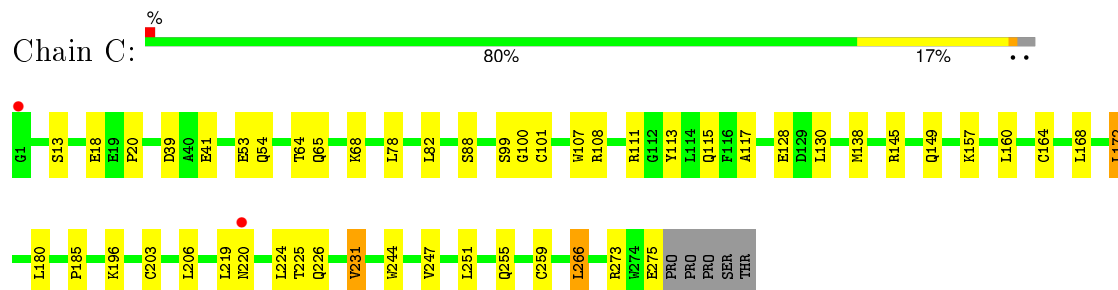
### 3 Residue-property plots

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

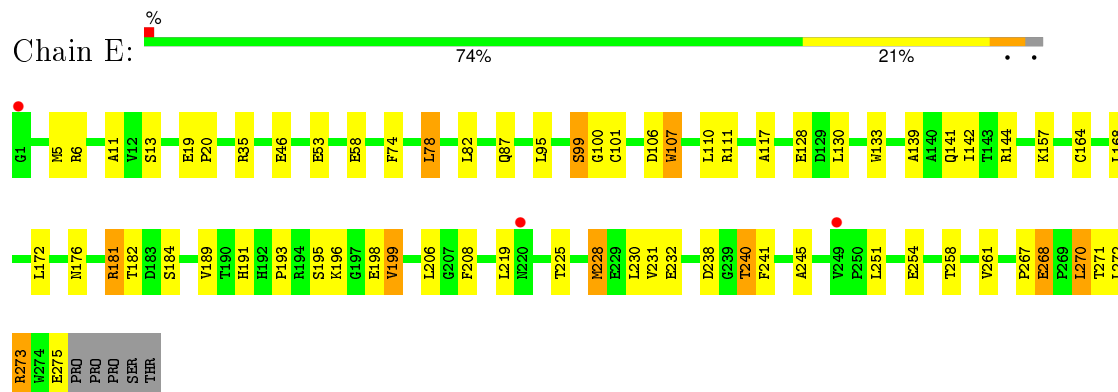
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



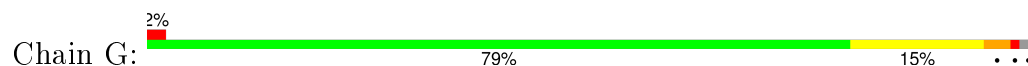
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

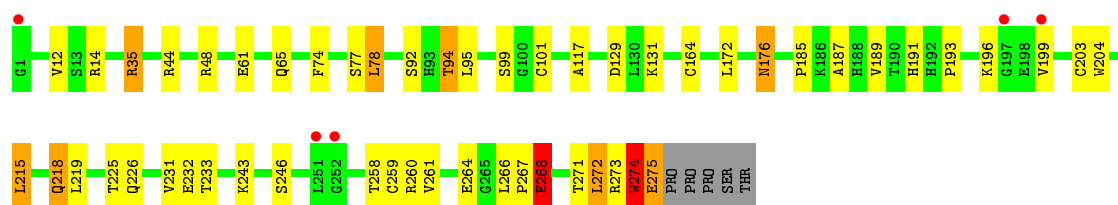


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain





- Molecule 2: Beta-2-microglobulin

Chain B: 84% 14%



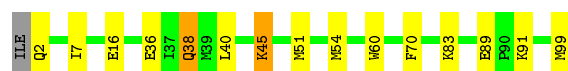
- Molecule 2: Beta-2-microglobulin

Chain D: 78% 20%



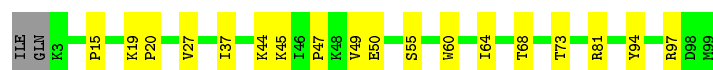
- Molecule 2: Beta-2-microglobulin

Chain F: 84% 13%



- Molecule 2: Beta-2-microglobulin

Chain H: 80% 18%



- Molecule 3: NP-N3D peptide

Chain I: 67% 11% 22%



- Molecule 3: NP-N3D peptide

Chain J: 78% 22%



- Molecule 3: NP-N3D peptide

Chain K: 78% 22%





- Molecule 3: NP-N3D peptide

Chain L:  67% 22% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.57Å 85.46Å 138.51Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	59.01 – 2.80 59.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.01-2.80) 99.8 (59.01-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.186 , 0.258 0.197 , 0.277	Depositor DCC
$R_{free}$ test set	2382 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.9	EDS
Estimated twinning fraction	0.001 for -k,-h,-l 0.003 for k,h,-l 0.023 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 47090 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12637	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	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 28.25 % 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 1.9035e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.51	0/2323	0.76	0/3154
1	C	0.52	0/2323	0.76	0/3154
1	E	0.54	0/2323	0.75	0/3154
1	G	0.50	0/2323	0.75	0/3154
2	B	0.55	0/827	0.77	0/1121
2	D	0.56	0/827	0.77	0/1121
2	F	0.56	0/836	0.76	0/1133
2	H	0.51	0/827	0.74	0/1121
3	I	0.63	0/68	1.04	0/88
3	J	0.53	0/68	0.71	0/88
3	K	0.63	0/68	0.96	0/88
3	L	0.53	0/68	0.80	0/88
All	All	0.53	0/12881	0.76	0/17464

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2257	0	2133	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2257	0	2133	13	0
1	E	2257	0	2133	28	0
1	G	2257	0	2133	25	0
2	B	801	0	777	5	0
2	D	801	0	775	9	0
2	F	810	0	785	4	0
2	H	801	0	777	6	0
3	I	69	0	59	1	0
3	J	69	0	59	0	0
3	K	69	0	59	0	0
3	L	69	0	59	3	0
4	A	5	0	0	0	0
4	C	10	0	0	0	0
4	E	10	0	0	0	0
5	A	15	0	0	0	0
5	B	8	0	0	0	0
5	C	15	0	0	1	0
5	D	10	0	0	1	0
5	E	19	0	0	0	0
5	F	17	0	0	0	0
5	G	8	0	0	0	0
5	H	3	0	0	0	0
All	All	12637	0	11882	100	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 4.

All (100) 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:G:185:PRO:HD2	1:G:266:LEU:HD13	1.53	0.90
1:G:77:SER:HB3	3:L:9:MET:HG3	1.62	0.80
1:A:101:CYS:HG	1:A:164:CYS:HG	0.76	0.74
1:C:101:CYS:HG	1:C:164:CYS:HG	0.72	0.69
2:F:38:GLN:HG3	2:F:45:LYS:HE2	1.74	0.69
1:A:215:LEU:HD22	1:A:261:VAL:HG22	1.76	0.67
1:C:203:CYS:HG	1:C:259:CYS:HG	0.72	0.67
3:I:6:MET:HG3	3:I:7:GLU:H	1.61	0.66
3:L:6:MET:HG3	3:L:7:GLU:H	1.61	0.65
1:G:193:PRO:HA	1:G:199:VAL:HG22	1.77	0.65
2:H:15:PRO:HG3	2:H:97:ARG:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.35	0.61
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.83	0.59
1:E:130:LEU:HB2	1:E:157:LYS:HG3	1.84	0.59
1:E:189:VAL:HG23	1:E:272:LEU:HD23	1.83	0.59
1:E:82:LEU:HD12	1:E:87:GLN:HB2	1.85	0.57
2:D:17:ASN:HD21	2:D:74:GLU:HG2	1.69	0.57
1:G:189:VAL:HG23	1:G:272:LEU:HD12	1.87	0.57
2:D:24:ASN:HB3	2:D:65:LEU:HD11	1.87	0.56
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.87	0.56
1:G:61:GLU:O	1:G:65:GLN:HG2	2.06	0.55
1:E:191:HIS:HE1	1:E:254:GLU:HG2	1.72	0.55
1:G:95:LEU:HD21	3:L:9:MET:HE3	1.89	0.54
1:C:185:PRO:HD2	1:C:266:LEU:HD13	1.89	0.53
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.88	0.53
2:D:37:ILE:HG12	2:D:82:VAL:HG22	1.92	0.52
1:G:274:TRP:O	1:G:275:GLU:HB2	2.10	0.52
1:E:258:THR:OG1	1:E:273:ARG:HD2	2.11	0.51
1:E:261:VAL:HB	1:E:270:LEU:HB2	1.92	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.50
1:C:64:THR:O	1:C:68:LYS:HG2	2.12	0.50
1:A:203:CYS:HG	1:A:259:CYS:HG	1.02	0.50
1:G:74:PHE:O	1:G:78:LEU:HB2	2.12	0.49
1:C:108:ARG:HD2	5:C:414:HOH:O	2.11	0.49
2:F:36:GLU:HB2	2:F:83:LYS:HB2	1.94	0.49
1:A:219:LEU:HG	1:A:257:TYR:CE2	2.47	0.49
2:D:20:PRO:HD3	1:E:181:ARG:HD3	1.95	0.49
1:G:129:ASP:HB2	1:G:131:LYS:HE3	1.95	0.49
1:C:168:LEU:HG	1:C:172:LEU:HD12	1.95	0.49
1:E:74:PHE:O	1:E:78:LEU:HB2	2.14	0.48
1:G:215:LEU:HD22	1:G:261:VAL:HG22	1.94	0.48
2:H:49:VAL:HG22	2:H:68:THR:HB	1.96	0.48
1:E:228:MET:HE1	1:E:245:ALA:HB1	1.95	0.48
2:B:33:PRO:HD3	2:B:62:PHE:CE1	2.48	0.47
1:E:78:LEU:HD13	1:E:95:LEU:HB2	1.96	0.47
1:G:172:LEU:O	1:G:176:ASN:HB3	2.14	0.47
1:A:219:LEU:HB2	1:A:224:LEU:HD21	1.97	0.47
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.50	0.46
1:G:101:CYS:HG	1:G:164:CYS:HG	0.53	0.46
1:C:130:LEU:HB2	1:C:157:LYS:HG3	1.97	0.46
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.51	0.46
1:E:208:PHE:CE1	1:E:241:PHE:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:PRO:O	1:G:268:GLU:HB3	2.16	0.46
1:G:187:ALA:HA	1:G:204:TRP:O	2.15	0.46
1:E:5:MET:HB2	1:E:168:LEU:HD13	1.98	0.45
1:E:267:PRO:O	1:E:268:GLU:HB3	2.16	0.45
1:G:35:ARG:HB3	1:G:48:ARG:HD3	1.98	0.45
1:C:13:SER:HA	1:C:20:PRO:HB3	1.99	0.45
1:A:47:PRO:HB3	1:A:52:MET:HB3	1.97	0.45
1:E:139:ALA:HA	1:E:142:ILE:HD12	1.98	0.45
1:A:142:ILE:O	1:A:146:LYS:HB2	2.16	0.45
1:G:12:VAL:HG22	1:G:94:THR:HG23	1.99	0.45
1:C:100:GLY:O	1:C:160:LEU:HD22	2.17	0.45
1:E:11:ALA:HB2	1:E:74:PHE:HB3	1.99	0.45
1:E:181:ARG:HG2	1:E:182:THR:H	1.82	0.45
1:E:13:SER:HA	1:E:20:PRO:HB3	2.00	0.44
1:E:191:HIS:NE2	1:E:199:VAL:HG21	2.32	0.44
1:G:233:THR:OG1	1:G:243:LYS:HD2	2.17	0.44
1:G:274:TRP:HD1	1:G:275:GLU:N	2.15	0.44
1:A:193:PRO:HA	1:A:199:VAL:HG22	1.99	0.44
1:E:101:CYS:CB	1:E:164:CYS:HG	2.27	0.44
1:C:107:TRP:CH2	1:C:172:LEU:HB3	2.53	0.44
1:C:231:VAL:HG12	1:C:244:TRP:H	1.82	0.44
2:D:20:PRO:HD3	1:E:181:ARG:CD	2.49	0.43
2:D:38:GLN:HG2	2:D:45:LYS:HE2	1.99	0.43
2:D:3:LYS:HG2	5:D:110:HOH:O	2.18	0.43
2:H:27:VAL:HG21	2:H:37:ILE:HG12	2.00	0.43
1:E:238:ASP:OD1	1:E:240:THR:OG1	2.35	0.43
2:B:41:LYS:HB2	2:B:46:ILE:HD11	2.01	0.43
1:A:99:SER:HA	1:A:113:TYR:O	2.19	0.42
1:G:78:LEU:HD13	1:G:95:LEU:HB2	2.02	0.42
1:G:203:CYS:HG	1:G:259:CYS:HG	0.45	0.42
1:A:249:VAL:HB	1:A:257:TYR:CE1	2.55	0.42
1:E:133:TRP:HB2	1:E:144:ARG:HG3	2.01	0.42
1:G:191:HIS:CE1	1:G:199:VAL:HG11	2.55	0.42
1:G:274:TRP:CD1	1:G:275:GLU:N	2.88	0.42
1:E:5:MET:O	1:E:100:GLY:HA3	2.20	0.41
1:G:260:ARG:HH21	1:G:271:THR:HB	1.85	0.41
1:G:218:GLN:HG3	1:G:258:THR:O	2.21	0.41
1:C:99:SER:HA	1:C:113:TYR:O	2.19	0.41
2:B:79:ALA:HB2	2:B:94:TYR:CD2	2.55	0.41
1:E:6:ARG:HA	1:E:99:SER:O	2.21	0.41
1:E:11:ALA:CB	1:E:74:PHE:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:PRO:HA	2:D:15:PRO:HD3	1.94	0.41
2:H:94:TYR:N	2:H:94:TYR:CD1	2.88	0.41
2:F:7:ILE:HD12	2:F:91:LYS:HG2	2.02	0.41
2:H:19:LYS:HA	2:H:20:PRO:HD3	1.98	0.40
1:A:189:VAL:HG22	1:A:203:CYS:HB2	2.02	0.40
1:E:19:GLU:HA	1:E:20:PRO:HD3	1.93	0.40
1:E:107:TRP:CH2	1:E:172:LEU:HB3	2.57	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	273/280 (98%)	256 (94%)	16 (6%)	1 (0%)	39	74
1	C	273/280 (98%)	265 (97%)	6 (2%)	2 (1%)	26	62
1	E	273/280 (98%)	259 (95%)	11 (4%)	3 (1%)	17	50
1	G	273/280 (98%)	254 (93%)	16 (6%)	3 (1%)	17	50
2	B	95/99 (96%)	91 (96%)	4 (4%)	0	100	100
2	D	95/99 (96%)	90 (95%)	5 (5%)	0	100	100
2	F	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
2	H	95/99 (96%)	91 (96%)	4 (4%)	0	100	100
3	I	7/9 (78%)	6 (86%)	0	1 (14%)	0	1
3	J	7/9 (78%)	6 (86%)	0	1 (14%)	0	1
3	K	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	L	7/9 (78%)	6 (86%)	0	1 (14%)	0	1
All	All	1501/1552 (97%)	1420 (95%)	69 (5%)	12 (1%)	24	58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	268	GLU
1	G	176	ASN
1	G	274	TRP
1	E	107	TRP
3	J	7	GLU
3	L	6	MET
1	E	193	PRO
3	I	6	MET
1	C	54	GLN
1	C	128	GLU
1	A	268	GLU
1	G	268	GLU

### 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	233/238 (98%)	210 (90%)	23 (10%)	10	28
1	C	233/238 (98%)	204 (88%)	29 (12%)	6	17
1	E	233/238 (98%)	202 (87%)	31 (13%)	5	14
1	G	233/238 (98%)	211 (91%)	22 (9%)	11	31
2	B	91/93 (98%)	86 (94%)	5 (6%)	27	59
2	D	91/93 (98%)	84 (92%)	7 (8%)	16	41
2	F	92/93 (99%)	82 (89%)	10 (11%)	8	23
2	H	91/93 (98%)	83 (91%)	8 (9%)	12	35
3	I	8/8 (100%)	6 (75%)	2 (25%)	1	2
3	J	8/8 (100%)	7 (88%)	1 (12%)	6	17
3	K	8/8 (100%)	6 (75%)	2 (25%)	1	2
3	L	8/8 (100%)	8 (100%)	0	100	100
All	All	1329/1356 (98%)	1189 (90%)	140 (10%)	8	24

All (140) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	14	ARG
1	A	35	ARG
1	A	39	ASP
1	A	46	GLU
1	A	53	GLU
1	A	58	GLU
1	A	78	LEU
1	A	111	ARG
1	A	128	GLU
1	A	138	MET
1	A	149	GLN
1	A	178	THR
1	A	183	ASP
1	A	196	LYS
1	A	201	LEU
1	A	203	CYS
1	A	219	LEU
1	A	226	GLN
1	A	231	VAL
1	A	246	SER
1	A	255	GLN
1	A	258	THR
1	A	272	LEU
2	B	58	LYS
2	B	64	ILE
2	B	70	PHE
2	B	73	THR
2	B	75	THR
1	C	18	GLU
1	C	39	ASP
1	C	41	GLU
1	C	53	GLU
1	C	65	GLN
1	C	78	LEU
1	C	82	LEU
1	C	88	SER
1	C	111	ARG
1	C	115	GLN
1	C	138	MET
1	C	145	ARG
1	C	149	GLN
1	C	172	LEU
1	C	180	LEU

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Mol	Chain	Res	Type
1	C	196	LYS
1	C	206	LEU
1	C	219	LEU
1	C	220	ASN
1	C	224	LEU
1	C	225	THR
1	C	226	GLN
1	C	231	VAL
1	C	247	VAL
1	C	251	LEU
1	C	255	GLN
1	C	266	LEU
1	C	273	ARG
1	C	275	GLU
2	D	7	ILE
2	D	48	LYS
2	D	64	ILE
2	D	68	THR
2	D	70	PHE
2	D	83	LYS
2	D	91	LYS
1	E	35	ARG
1	E	46	GLU
1	E	53	GLU
1	E	58	GLU
1	E	78	LEU
1	E	99	SER
1	E	106	ASP
1	E	110	LEU
1	E	111	ARG
1	E	128	GLU
1	E	141	GLN
1	E	176	ASN
1	E	181	ARG
1	E	184	SER
1	E	195	SER
1	E	196	LYS
1	E	198	GLU
1	E	199	VAL
1	E	206	LEU
1	E	219	LEU
1	E	225	THR

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Mol	Chain	Res	Type
1	E	228	MET
1	E	230	LEU
1	E	231	VAL
1	E	232	GLU
1	E	240	THR
1	E	251	LEU
1	E	270	LEU
1	E	271	THR
1	E	273	ARG
1	E	275	GLU
2	F	2	GLN
2	F	16	GLU
2	F	38	GLN
2	F	40	LEU
2	F	45	LYS
2	F	51	MET
2	F	54	MET
2	F	70	PHE
2	F	89	GLU
2	F	99	MET
1	G	14	ARG
1	G	35	ARG
1	G	44	ARG
1	G	78	LEU
1	G	92	SER
1	G	94	THR
1	G	99	SER
1	G	196	LYS
1	G	215	LEU
1	G	218	GLN
1	G	219	LEU
1	G	225	THR
1	G	226	GLN
1	G	231	VAL
1	G	232	GLU
1	G	246	SER
1	G	264	GLU
1	G	268	GLU
1	G	272	LEU
1	G	273	ARG
1	G	274	TRP
1	G	275	GLU

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Mol	Chain	Res	Type
2	H	44	LYS
2	H	45	LYS
2	H	47	PRO
2	H	50	GLU
2	H	55	SER
2	H	64	ILE
2	H	73	THR
2	H	81	ARG
3	I	7	GLU
3	I	8	THR
3	J	6	MET
3	K	2	SER
3	K	7	GLU

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

Mol	Chain	Res	Type
1	A	149	GLN
1	A	255	GLN
1	C	80	ASN
2	D	17	ASN
2	D	29	GLN
1	G	127	ASN
2	H	42	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	301	-	4,4,4	0.12	0	6,6,6	0.14	0
4	SO4	C	301	-	4,4,4	0.20	0	6,6,6	0.25	0
4	SO4	C	302	-	4,4,4	0.05	0	6,6,6	0.19	0
4	SO4	E	301	-	4,4,4	0.34	0	6,6,6	0.30	0
4	SO4	E	302	-	4,4,4	0.15	0	6,6,6	0.29	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	SO4	A	301	-	-	0/0/0/0	0/0/0/0
4	SO4	C	301	-	-	0/0/0/0	0/0/0/0
4	SO4	C	302	-	-	0/0/0/0	0/0/0/0
4	SO4	E	301	-	-	0/0/0/0	0/0/0/0
4	SO4	E	302	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/280 (98%)	-0.12	0 100 100	28, 53, 87, 109	1 (0%)
1	C	275/280 (98%)	-0.14	2 (0%) 89 84	33, 51, 83, 103	4 (1%)
1	E	275/280 (98%)	-0.19	3 (1%) 82 74	22, 44, 86, 119	1 (0%)
1	G	275/280 (98%)	-0.01	5 (1%) 71 61	37, 57, 97, 112	0
2	B	97/99 (97%)	-0.31	0 100 100	22, 47, 74, 79	0
2	D	97/99 (97%)	-0.32	0 100 100	28, 48, 72, 81	1 (1%)
2	F	98/99 (98%)	-0.31	0 100 100	25, 43, 65, 89	0
2	H	97/99 (97%)	-0.26	0 100 100	36, 58, 78, 96	0
3	I	9/9 (100%)	0.05	0 100 100	47, 53, 66, 71	0
3	J	9/9 (100%)	0.32	0 100 100	48, 56, 69, 72	0
3	K	9/9 (100%)	-0.04	0 100 100	36, 38, 50, 59	0
3	L	9/9 (100%)	0.39	0 100 100	58, 66, 71, 73	0
All	All	1525/1552 (98%)	-0.16	10 (0%) 89 84	22, 51, 86, 119	7 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	252	GLY	3.7
1	G	251	LEU	3.0
1	G	1	GLY	2.9
1	C	1	GLY	2.9
1	G	199	VAL	2.8
1	G	197	GLY	2.7
1	E	1	GLY	2.6
1	C	220	ASN	2.6
1	E	249	VAL	2.1
1	E	220	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	E	301	5/5	0.98	0.17	0.07	52,55,59,61	0
4	SO4	C	301	5/5	0.95	0.16	-0.61	80,82,83,85	0
4	SO4	C	302	5/5	0.96	0.19	-	88,91,93,93	0
4	SO4	E	302	5/5	0.89	0.25	-	100,102,104,105	0
4	SO4	A	301	5/5	0.95	0.16	-	92,93,94,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.