



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 01:51 PM JST

PDB ID : 5IJK  
Title : Crystal structure of anti-gliadin 1002-1E03 Fab fragment in complex of peptide PLQPEQFPF  
Authors : Snir, O.; Chen, X.; Gidoni, M.; du Pre, M.F.; Zhao, Y.; Steinsbo, O.; Lundin, K.E.; Yaari, G.; Sollid, L.M.  
Deposited on : 2016-03-02  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

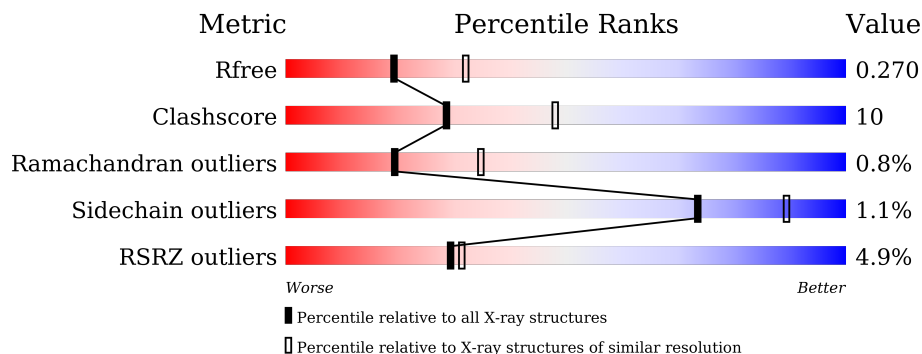
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	X	9	
1	Y	9	
2	A	228	
2	B	228	
3	C	221	
3	D	221	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6812 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 peptide PRO-LEU-GLN-PRO-GLU-GLN-PRO-PHE-PRO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	X	8	67	45	10	12	0	0	0
1	Y	9	74	50	11	13	0	0	0

- Molecule 2 is a protein called 1E03 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	213	1594	1012	266	311	5	0	0	0
2	B	211	1584	1007	264	308	5	0	0	0

- Molecule 3 is a protein called 1E03 Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	218	1691	1062	283	341	5	0	0	0
3	D	218	1691	1062	283	341	5	0	0	0

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		

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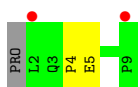
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	B	5	Total O 5 5	0	0
5	C	24	Total O 24 24	0	0
5	D	9	Total O 9 9	0	0

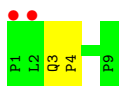
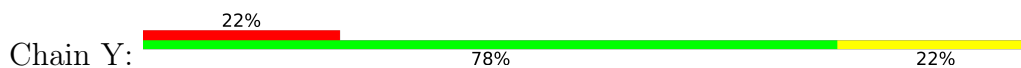
### 3 Residue-property plots

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.

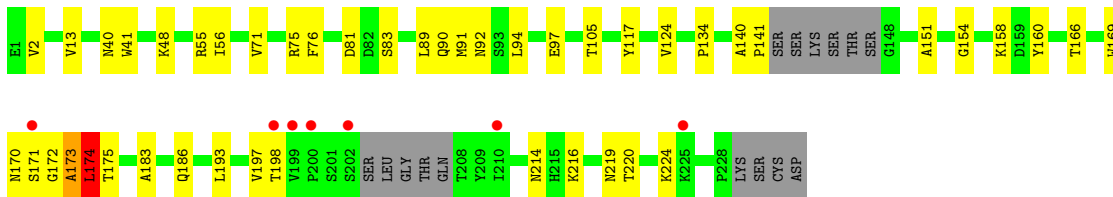
- Molecule 1: peptide PRO-LEU-GLN-PRO-GLU-GLN-PRO-PHE-PRO



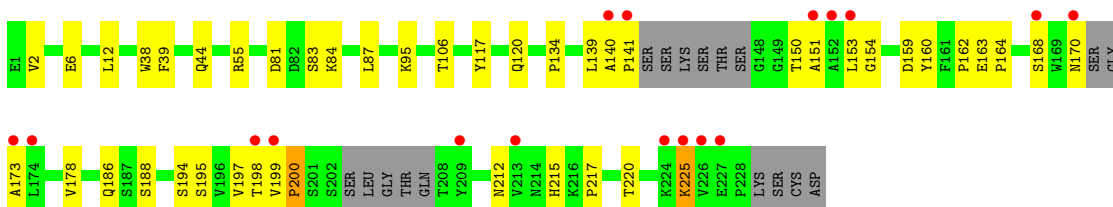
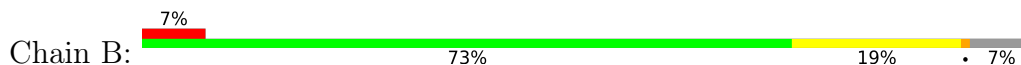
- Molecule 1: peptide PRO-LEU-GLN-PRO-GLU-GLN-PRO-PHE-PRO




- Molecule 2: 1E03 Fab fragment heavy chain

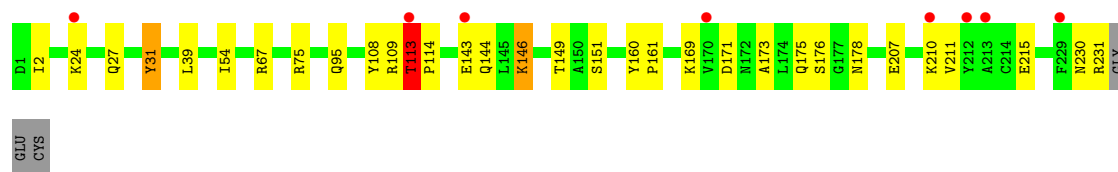


- Molecule 2: 1E03 Fab fragment heavy chain




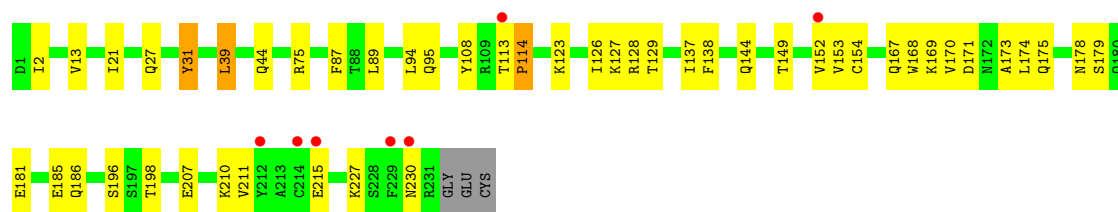
- Molecule 3: 1E03 Fab fragment light chain

Chain C:  4% 84% 13% ..



- Molecule 3: 1E03 Fab fragment light chain

Chain D:  3% 77% 20% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.64Å 144.64Å 106.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 2.50 47.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.29-2.50) 92.8 (47.29-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.209 , 0.265 0.219 , 0.270	Depositor DCC
$R_{free}$ test set	1991 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtrriage
Anisotropy	0.453	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	X	0.38	0/70	0.62	0/96
1	Y	0.33	0/78	0.52	0/107
2	A	0.34	0/1632	0.64	1/2227 (0.0%)
2	B	0.36	0/1621	0.64	2/2211 (0.1%)
3	C	0.32	0/1729	0.62	1/2351 (0.0%)
3	D	0.40	2/1729 (0.1%)	0.63	0/2351
All	All	0.36	2/6859 (0.0%)	0.63	4/9343 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	215	GLU	CD-OE1	-7.43	1.17	1.25
3	D	215	GLU	CD-OE2	-6.15	1.18	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	113	THR	C-N-CD	9.88	149.14	128.40
2	B	95	LYS	CB-CA-C	5.23	120.86	110.40
2	A	174	LEU	N-CA-C	5.14	124.87	111.00
2	B	95	LYS	N-CA-CB	-5.09	101.44	110.60

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	X	67	0	62	4	0
1	Y	74	0	72	1	0
2	A	1594	0	1568	33	1
2	B	1584	0	1559	43	1
3	C	1691	0	1646	24	0
3	D	1691	0	1646	33	1
4	A	15	0	0	0	0
4	B	10	0	0	0	1
4	C	10	0	0	0	0
4	D	20	0	0	0	0
5	A	18	0	0	1	0
5	B	5	0	0	0	0
5	C	24	0	0	1	0
5	D	9	0	0	0	0
All	All	6812	0	6553	129	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (129) 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)
2:B:170:ASN:C	2:B:173:ALA:CB	2.01	1.29
2:B:170:ASN:CB	2:B:173:ALA:HA	1.65	1.27
2:B:170:ASN:C	2:B:173:ALA:HB2	1.60	1.21
2:B:170:ASN:HB2	2:B:173:ALA:CA	1.86	1.06
2:B:170:ASN:HB2	2:B:173:ALA:HA	1.06	1.02
3:D:126:ILE:H	3:D:186:GLN:HE22	1.15	0.93
2:B:170:ASN:C	2:B:173:ALA:CA	2.38	0.92
3:C:210:LYS:HE3	3:C:230:ASN:HB3	1.52	0.90
2:B:170:ASN:CA	2:B:173:ALA:HA	2.02	0.89
1:X:5:GLU:OE2	3:C:113:THR:OG1	1.91	0.88
2:B:170:ASN:C	2:B:173:ALA:HA	1.94	0.88
2:A:214:ASN:HD21	2:A:216:LYS:HD3	1.40	0.84
3:D:173:ALA:O	3:D:175:GLN:NE2	2.11	0.83
2:B:6:GLU:H	2:B:120:GLN:HE22	1.23	0.83
3:C:169:LYS:NZ	3:C:215:GLU:OE1	2.14	0.79
3:D:123:LYS:NZ	3:D:185:GLU:OE2	2.13	0.78
2:B:170:ASN:C	2:B:173:ALA:HB1	2.03	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ASN:CB	2:B:173:ALA:CA	2.54	0.75
3:C:95:GLN:OE1	3:D:75:ARG:NH1	2.18	0.73
2:B:225:LYS:HD3	2:B:225:LYS:H	1.53	0.72
3:D:210:LYS:HD3	3:D:230:ASN:HB2	1.73	0.71
1:X:4:PRO:HA	5:C:401:HOH:O	1.89	0.71
3:C:31:TYR:HB2	3:C:108:TYR:HE1	1.56	0.69
2:B:168:SER:OG	2:B:212:ASN:OD1	2.09	0.68
3:D:126:ILE:H	3:D:186:GLN:NE2	1.89	0.67
2:B:170:ASN:O	2:B:173:ALA:HB2	1.96	0.65
2:A:214:ASN:OD1	2:A:216:LYS:NZ	2.25	0.64
3:D:31:TYR:HB2	3:D:108:TYR:HE1	1.62	0.64
2:A:197:VAL:HG22	2:A:198:THR:H	1.63	0.63
2:A:214:ASN:HD21	2:A:216:LYS:CD	2.12	0.62
3:C:173:ALA:O	3:C:175:GLN:NE2	2.29	0.62
3:D:211:VAL:HG12	3:D:230:ASN:HB3	1.82	0.61
3:C:113:THR:HG23	3:C:114:PRO:CD	2.31	0.61
3:D:154:CYS:HB2	3:D:168:TRP:CH2	2.36	0.61
2:B:44:GLN:HE22	3:D:44:GLN:HE22	1.48	0.60
3:D:126:ILE:N	3:D:186:GLN:HE22	1.93	0.60
2:B:6:GLU:H	2:B:120:GLN:NE2	1.98	0.60
3:C:144:GLN:HG2	3:C:149:THR:O	2.04	0.58
2:A:71:VAL:HG13	2:A:76:PHE:CG	2.40	0.56
3:D:169:LYS:HG2	3:D:174:LEU:HA	1.89	0.55
2:B:150:THR:HA	2:B:200:PRO:HD3	1.88	0.55
1:X:5:GLU:OE2	2:A:55:ARG:NH2	2.39	0.54
2:B:178:VAL:HG22	2:B:197:VAL:HG12	1.90	0.54
3:D:21:ILE:HD11	3:D:89:LEU:HD23	1.89	0.54
2:B:198:THR:O	2:B:199:VAL:HG12	2.08	0.53
2:A:48:LYS:O	5:A:401:HOH:O	2.18	0.53
3:C:143:GLU:N	3:C:143:GLU:OE1	2.40	0.53
2:B:38:TRP:CZ3	2:B:55:ARG:NH1	2.76	0.53
3:C:143:GLU:HA	3:C:146:LYS:HE2	1.89	0.53
3:C:109:ARG:HG3	3:C:109:ARG:NH1	2.24	0.52
2:B:215:HIS:CD2	2:B:217:PRO:HD2	2.45	0.52
2:A:41:TRP:CE2	2:A:89:LEU:HB2	2.45	0.52
2:B:38:TRP:CE3	2:B:55:ARG:NH1	2.78	0.51
2:B:153:LEU:HG	2:B:197:VAL:HG22	1.93	0.51
2:A:170:ASN:C	2:A:172:GLY:HA2	2.31	0.51
3:C:109:ARG:HG3	3:C:109:ARG:HH11	1.76	0.51
2:A:173:ALA:HA	2:A:174:LEU:C	2.31	0.51
3:C:210:LYS:HZ1	3:C:231:ARG:HG3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:39:LEU:HD13	3:D:87:PHE:CD1	2.46	0.50
3:D:13:VAL:CG2	3:D:94:LEU:HD22	2.43	0.49
3:D:170:VAL:H	3:D:175:GLN:HE21	1.59	0.49
2:A:40:ASN:HB2	2:A:105:THR:HG23	1.95	0.49
2:B:38:TRP:O	2:B:106:THR:OG1	2.24	0.49
3:D:178:ASN:OD1	3:D:178:ASN:N	2.45	0.49
2:A:158:LYS:NZ	2:A:186:GLN:OE1	2.46	0.48
3:C:178:ASN:N	3:C:178:ASN:OD1	2.47	0.48
2:A:97:GLU:OE1	2:A:97:GLU:N	2.37	0.48
3:D:210:LYS:CD	3:D:230:ASN:HB2	2.42	0.48
3:D:207:GLU:HA	3:D:207:GLU:OE2	2.14	0.47
2:A:2:VAL:HG21	2:A:117:TYR:CZ	2.48	0.47
2:A:71:VAL:HG13	2:A:76:PHE:HB2	1.96	0.47
2:B:159:ASP:OD1	2:B:186:GLN:NE2	2.29	0.47
2:A:134:PRO:HD2	2:A:220:THR:HG21	1.95	0.47
2:B:140:ALA:HB1	2:B:141:PRO:HA	1.95	0.47
2:A:171:SER:O	2:B:168:SER:OG	2.33	0.47
3:D:137:ILE:HG22	3:D:227:LYS:HG2	1.97	0.47
2:A:2:VAL:HG11	2:A:117:TYR:CG	2.50	0.47
3:C:230:ASN:O	3:C:231:ARG:HB2	2.14	0.46
3:C:75:ARG:NH1	3:D:95:GLN:OE1	2.31	0.46
1:Y:3:GLN:HG2	1:Y:4:PRO:O	2.15	0.46
2:A:81:ASP:OD1	2:A:83:SER:OG	2.30	0.46
2:B:225:LYS:H	2:B:225:LYS:CD	2.24	0.45
3:C:113:THR:OG1	3:C:114:PRO:HD3	2.16	0.45
2:B:151:ALA:O	2:B:198:THR:HA	2.17	0.45
2:B:2:VAL:HG21	2:B:117:TYR:CZ	2.51	0.45
1:X:5:GLU:CD	3:C:113:THR:OG1	2.54	0.45
2:A:151:ALA:O	2:A:198:THR:HA	2.16	0.45
3:D:138:PHE:HB2	3:D:153:VAL:CG1	2.47	0.45
2:A:166:THR:CG2	2:A:214:ASN:HD22	2.30	0.44
2:B:139:LEU:HB3	3:D:138:PHE:CD2	2.52	0.44
2:B:163:GLU:CG	2:B:164:PRO:HA	2.47	0.44
3:D:179:SER:HA	3:D:198:THR:O	2.17	0.44
2:A:13:VAL:HG11	2:A:94:LEU:HD13	2.00	0.44
2:B:154:GLY:HA3	2:B:195:SER:O	2.18	0.44
2:A:55:ARG:HG2	2:A:56:ILE:N	2.33	0.43
2:A:173:ALA:HA	2:A:175:THR:HG23	2.00	0.43
2:B:12:LEU:HB2	2:B:162:PRO:HG3	2.00	0.43
3:D:113:THR:OG1	3:D:114:PRO:HD3	2.17	0.43
3:C:207:GLU:OE2	3:C:207:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2:ILE:HG12	3:D:27:GLN:HG2	2.01	0.43
2:B:163:GLU:HG3	2:B:164:PRO:HA	2.00	0.43
2:A:183:ALA:HA	2:A:193:LEU:HB3	1.99	0.43
3:D:171:ASP:HA	3:D:211:VAL:HG23	1.99	0.43
3:D:167:GLN:HB3	3:D:174:LEU:CD1	2.48	0.43
2:A:134:PRO:HB3	2:A:160:TYR:HB3	2.00	0.43
2:A:171:SER:N	2:A:172:GLY:HA2	2.34	0.42
2:B:2:VAL:HG11	2:B:117:TYR:CG	2.53	0.42
2:B:215:HIS:HB3	2:B:220:THR:OG1	2.19	0.42
2:A:71:VAL:CG1	2:A:76:PHE:HB2	2.50	0.42
3:D:128:ARG:NH1	3:D:129:THR:OG1	2.52	0.42
3:C:171:ASP:HA	3:C:211:VAL:CG2	2.50	0.42
2:B:39:PHE:HB3	2:B:87:LEU:HD22	2.02	0.42
2:A:224:LYS:HA	2:A:224:LYS:HD2	1.77	0.42
3:C:2:ILE:HG12	3:C:27:GLN:HG2	2.02	0.42
2:B:134:PRO:HB3	2:B:160:TYR:HB3	2.01	0.42
2:A:154:GLY:HA2	2:A:169:TRP:CH2	2.55	0.41
2:A:140:ALA:HB1	2:A:141:PRO:HA	2.02	0.41
2:A:75:ARG:HB3	2:A:92:ASN:O	2.21	0.41
3:C:54:ILE:HD13	3:C:67:ARG:HA	2.03	0.41
3:D:144:GLN:HG2	3:D:149:THR:O	2.20	0.41
2:B:139:LEU:HD22	3:D:153:VAL:HG11	2.02	0.41
3:C:144:GLN:HE22	3:C:151:SER:CB	2.34	0.41
2:B:81:ASP:OD1	2:B:83:SER:OG	2.31	0.41
2:B:163:GLU:OE2	2:B:164:PRO:HA	2.21	0.41
2:A:91:MET:HE1	2:A:124:VAL:HG21	2.03	0.40
3:C:160:TYR:CG	3:C:161:PRO:HA	2.57	0.40
2:B:81:ASP:OD2	2:B:84:LYS:HD3	2.22	0.40
3:D:152:VAL:HG12	3:D:168:TRP:CH2	2.56	0.40
3:D:181:GLU:HA	3:D:196:SER:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:SER:OG	2:B:188:SER:OG[7_555]	1.14	1.06
3:D:127:LYS:NZ	4:B:302:SO4:O1[3_445]	2.10	0.10
2:A:90:GLN:NE2	2:A:92:ASN:OD1[7_556]	2.11	0.09

## 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	X	6/9 (67%)	6 (100%)	0	0	100	100
1	Y	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	A	207/228 (91%)	198 (96%)	7 (3%)	2 (1%)	15	28
2	B	203/228 (89%)	197 (97%)	5 (2%)	1 (0%)	29	48
3	C	216/221 (98%)	202 (94%)	12 (6%)	2 (1%)	17	31
3	D	216/221 (98%)	202 (94%)	12 (6%)	2 (1%)	17	31
All	All	855/916 (93%)	811 (95%)	37 (4%)	7 (1%)	19	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	173	ALA
3	C	113	THR
2	A	174	LEU
3	C	31	TYR
3	D	31	TYR
2	B	200	PRO
3	D	114	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	X	8/9 (89%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	9/9 (100%)	9 (100%)	0	100	100
2	A	178/192 (93%)	177 (99%)	1 (1%)	86	95
2	B	177/192 (92%)	175 (99%)	2 (1%)	73	89
3	C	193/195 (99%)	189 (98%)	4 (2%)	53	78
3	D	193/195 (99%)	192 (100%)	1 (0%)	88	96
All	All	758/792 (96%)	750 (99%)	8 (1%)	73	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	219	ASN
2	B	194	SER
2	B	225	LYS
3	C	24	LYS
3	C	39	LEU
3	C	146	LYS
3	C	176	SER
3	D	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	44	GLN
2	B	120	GLN
3	C	158	ASN
3	C	167	GLN
3	D	186	GLN
3	D	219	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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	D	302	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	B	302	-	4,4,4	0.16	0	6,6,6	0.09	0
4	SO4	A	301	-	4,4,4	0.13	0	6,6,6	0.09	0
4	SO4	A	303	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	A	302	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	D	301	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	B	301	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	D	303	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	C	301	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	D	304	-	4,4,4	0.14	0	6,6,6	0.07	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	SO4	0	1



## 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<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	X	8/9 (88%)	0.81	2 (25%) 0 0	56, 59, 79, 91	0
1	Y	9/9 (100%)	1.95	2 (22%) 0 0	69, 76, 119, 128	0
2	A	213/228 (93%)	0.19	7 (3%) 46 50	42, 57, 82, 93	0
2	B	211/228 (92%)	0.42	17 (8%) 12 12	30, 71, 93, 105	0
3	C	218/221 (98%)	0.25	8 (3%) 41 45	40, 55, 88, 103	0
3	D	218/221 (98%)	0.33	7 (3%) 47 51	46, 65, 96, 103	0
All	All	877/916 (95%)	0.32	43 (4%) 29 31	30, 62, 92, 128	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	1	PRO	10.7
2	A	171	SER	4.7
3	D	212	TYR	4.1
2	A	199	VAL	3.9
2	B	152	ALA	3.8
1	X	2	LEU	3.6
2	B	209	TYR	3.6
2	B	224	LYS	3.6
2	A	202	SER	3.5
2	B	174	LEU	3.5
3	C	170	VAL	3.4
2	A	200	PRO	3.3
3	C	113	THR	3.3
3	C	210	LYS	3.2
3	C	229	PHE	3.1
2	B	199	VAL	2.9
2	B	225	LYS	2.9
2	B	173	ALA	2.9
2	A	198	THR	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	152	VAL	2.8
2	B	153	LEU	2.8
3	C	212	TYR	2.8
2	B	213	VAL	2.7
3	C	213	ALA	2.7
3	D	229	PHE	2.7
2	B	141	PRO	2.6
3	D	214	CYS	2.5
2	A	225	LYS	2.4
3	D	230	ASN	2.4
2	B	227	GLU	2.3
2	A	210	ILE	2.3
3	C	24	LYS	2.2
2	B	198	THR	2.2
2	B	226	VAL	2.2
2	B	151	ALA	2.2
2	B	140	ALA	2.2
2	B	170	ASN	2.2
2	B	168	SER	2.1
1	X	9	PRO	2.1
3	C	143	GLU	2.1
1	Y	2	LEU	2.0
3	D	113	THR	2.0
3	D	215	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	302	5/5	0.80	0.17	88,92,110,116	0
4	SO4	D	302	5/5	0.84	0.20	90,101,107,109	0
4	SO4	C	302	5/5	0.86	0.19	59,91,104,117	0
4	SO4	A	303	5/5	0.86	0.27	99,117,117,118	0
4	SO4	C	301	5/5	0.90	0.19	85,87,102,109	0
4	SO4	D	303	5/5	0.92	0.20	89,100,101,102	0
4	SO4	D	301	5/5	0.94	0.15	73,79,80,85	0
4	SO4	D	304	5/5	0.94	0.22	86,93,97,102	0
4	SO4	A	302	5/5	0.95	0.21	82,83,85,88	0
4	SO4	B	301	5/5	0.96	0.13	83,88,94,100	0
4	SO4	A	301	5/5	0.96	0.14	69,73,84,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.