Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 01:29 pm BST

PDB ID	:	4K71
Title	:	Crystal structure of a high affinity Human Serum Albumin variant bound to the Neonatal Fc Receptor
Authors	:	Schmidt, M.M.; Townson, S.A.; Andreucci, A.; Dombrowski, C.; Erbe, D.V.; King, B.; Kovalchin, J.T.; Masci, A.; Murillo, A.; Schirmer, E.B.; Furfine, E.S.; Barnes, T.M.
Deposited on	:	2013-04-16
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

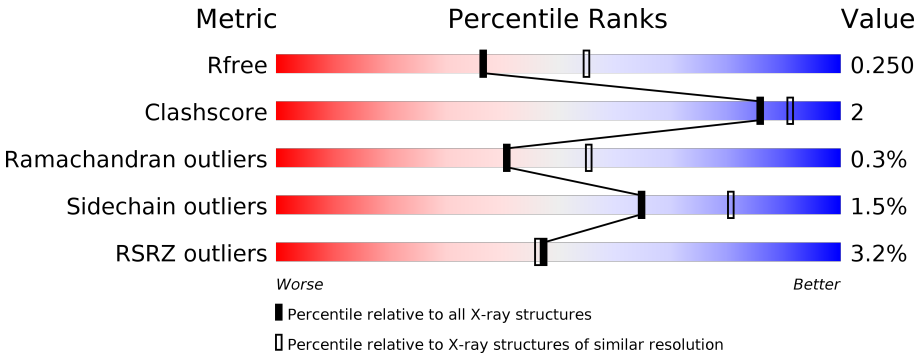
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	92% 7%
1	D	585	9% 92% 7%
2	B	274	90% 6%
2	E	274	90% 7%
3	C	99	94% 6%
3	F	99	92% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15259 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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	48	0	0
			4631	2923	784	882	42			
1	D	579	Total	C	N	O	S	107	0	0
			4597	2903	778	874	42			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	MET	VAL	ENGINEERED MUTATION	UNP P02768
A	420	ALA	THR	ENGINEERED MUTATION	UNP P02768
A	505	GLY	GLU	ENGINEERED MUTATION	UNP P02768
A	547	ALA	VAL	ENGINEERED MUTATION	UNP P02768
D	418	MET	VAL	ENGINEERED MUTATION	UNP P02768
D	420	ALA	THR	ENGINEERED MUTATION	UNP P02768
D	505	GLY	GLU	ENGINEERED MUTATION	UNP P02768
D	547	ALA	VAL	ENGINEERED MUTATION	UNP P02768

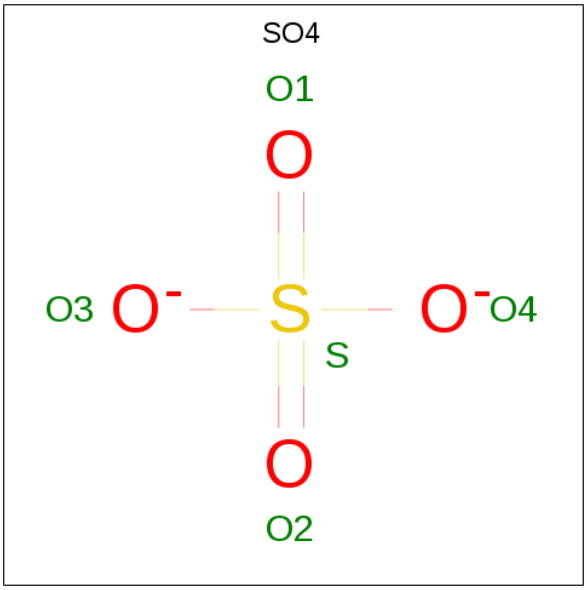
- Molecule 2 is a protein called IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	S	23	0	0
			2078	1329	358	383	8			
2	E	264	Total	C	N	O	S	10	0	0
			2078	1329	358	383	8			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	99	Total	C	N	O	S	23	0	0
			829	528	140	158	3			
3	F	99	Total	C	N	O	S	3	0	0
			829	528	140	158	3			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

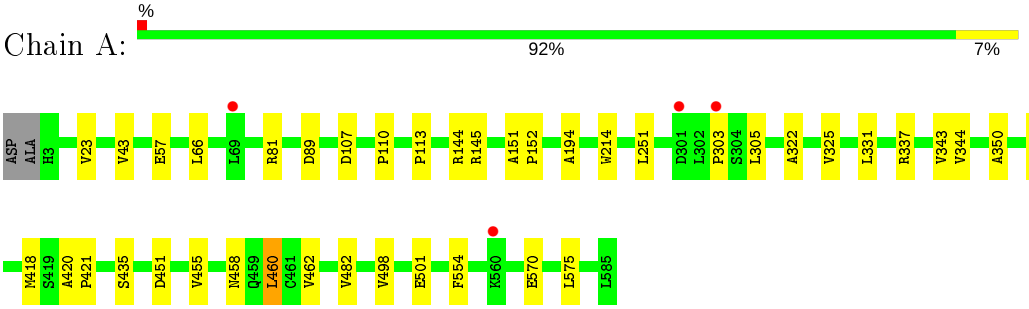
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	39	Total O 39 39	0	0
5	B	28	Total O 28 28	0	0
5	C	7	Total O 7 7	0	0
5	D	30	Total O 30 30	0	0
5	E	12	Total O 12 12	0	0
5	F	6	Total O 6 6	0	0

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 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.

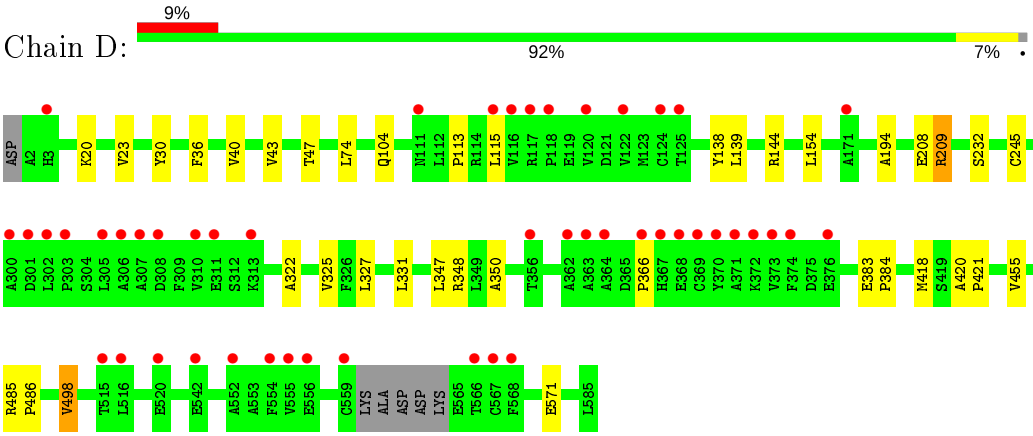
- Molecule 1: Serum albumin

Chain A:



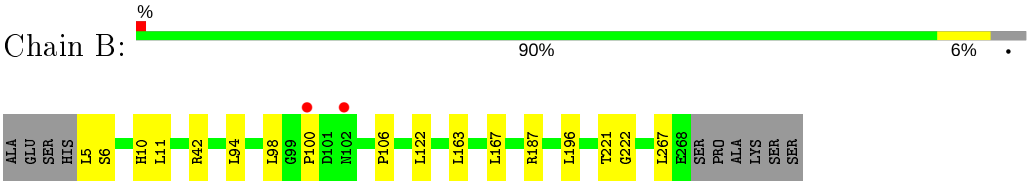
- Molecule 1: Serum albumin

Chain D:



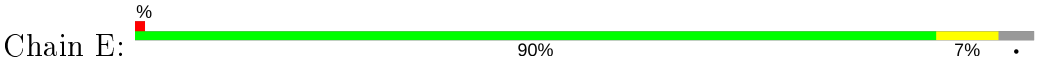
- Molecule 2: IgG receptor FcRn large subunit p51

Chain B:



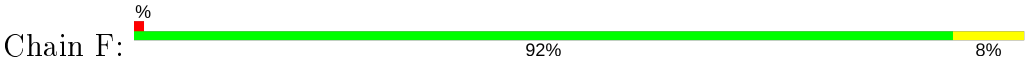
- Molecule 2: IgG receptor FcRn large subunit p51

Chain E:



• Molecule 3: Beta-2-microglobulin

• Molecule 3: Beta-2-microglobulin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	127.89Å 203.54Å 100.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.29 – 2.40 48.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (108.29-2.40) 99.8 (48.81-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.255 0.212 , 0.250	Depositor DCC
R_{free} test set	5144 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15259	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.67	0/4721	0.70	1/6364 (0.0%)
1	D	0.61	0/4686	0.68	3/6317 (0.0%)
2	B	0.69	0/2143	0.73	0/2912
2	E	0.64	0/2143	0.72	0/2912
3	C	0.67	0/852	0.76	0/1152
3	F	0.66	1/852 (0.1%)	0.74	0/1152
All	All	0.65	1/15397 (0.0%)	0.71	4/20809 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	80	CYS	CB-SG	-5.34	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	144	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	144	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	D	144	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	209	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4631	0	4554	24	0
1	D	4597	0	4519	20	0
2	B	2078	0	1989	10	0
2	E	2078	0	1989	9	0
3	C	829	0	794	3	0
3	F	829	0	794	2	0
4	A	35	0	0	1	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	30	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	A	39	0	0	1	0
5	B	28	0	0	0	0
5	C	7	0	0	0	0
5	D	30	0	0	0	0
5	E	12	0	0	0	0
5	F	6	0	0	1	0
All	All	15259	0	14639	64	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 2.

All (64) 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:5:LEU:HD23	2:B:167:LEU:HD21	1.69	0.75
1:D:331:LEU:HD13	1:D:350:ALA:HB2	1.70	0.73
1:A:81:ARG:NH2	1:A:89:ASP:OD1	2.27	0.67
2:B:98:LEU:HD13	2:B:163:LEU:HD23	1.78	0.66
3:F:31:HIS:ND1	5:F:205:HOH:O	2.28	0.66
1:A:498:VAL:HG23	2:B:42:ARG:NH1	2.11	0.66
1:A:305:LEU:HD11	1:A:337:ARG:HD2	1.82	0.62
1:A:331:LEU:HD13	1:A:350:ALA:HB2	1.83	0.61
1:D:418:MET:CE	1:D:460:LEU:HD11	2.31	0.60
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.35	0.60
2:B:106:PRO:HG2	2:B:122:LEU:HD13	1.86	0.58
1:D:23:VAL:HG12	1:D:43:VAL:HG22	1.86	0.56
1:A:498:VAL:HG23	2:B:42:ARG:HH12	1.70	0.55
1:D:20:LYS:HE3	1:D:47:THR:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ALA:HB1	1:D:325:VAL:HB	1.90	0.53
1:D:498:VAL:HG13	2:E:42:ARG:HH12	1.72	0.53
1:A:303:PRO:O	1:A:337:ARG:NH2	2.37	0.53
1:D:418:MET:HE2	1:D:460:LEU:HD11	1.92	0.52
3:F:25:CYS:HB2	3:F:39:LEU:HD21	1.91	0.52
1:D:498:VAL:HG13	2:E:42:ARG:NH1	2.24	0.52
1:A:66:LEU:HD13	1:A:251:LEU:HD12	1.92	0.51
1:A:305:LEU:HD11	1:A:337:ARG:CD	2.40	0.51
1:A:194:ALA:HB1	1:A:455:VAL:HG13	1.92	0.51
1:D:418:MET:HE1	1:D:460:LEU:HD11	1.92	0.51
1:D:383:GLU:HB3	1:D:384:PRO:HD3	1.93	0.50
1:A:498:VAL:HG22	5:A:714:HOH:O	2.10	0.50
2:B:221:THR:HG23	2:B:222:GLY:O	2.12	0.50
1:D:30:TYR:CD2	1:D:74:LEU:HD11	2.47	0.50
1:A:420:ALA:HB3	1:A:421:PRO:HD3	1.95	0.48
2:B:11:LEU:HD13	2:B:94:LEU:HD13	1.95	0.48
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.96	0.48
2:B:5:LEU:HD12	2:B:6:SER:H	1.79	0.48
1:D:194:ALA:HB1	1:D:455:VAL:CG1	2.44	0.47
1:D:331:LEU:HD21	1:D:347:LEU:CD2	2.44	0.47
2:B:98:LEU:HD13	2:B:163:LEU:CD2	2.43	0.47
1:D:20:LYS:CE	1:D:47:THR:HG21	2.44	0.47
2:E:186:ALA:HB2	2:E:196:LEU:CD1	2.45	0.46
1:D:36:PHE:CZ	1:D:40:VAL:HG21	2.51	0.46
1:A:113:PRO:O	1:A:145:ARG:NH1	2.48	0.45
2:E:54:GLU:OE2	2:E:166:HIS:ND1	2.38	0.44
1:A:458:ASN:O	1:A:462:VAL:HG13	2.17	0.44
1:D:209:ARG:NH2	1:D:327:LEU:HD13	2.32	0.44
3:C:64:LEU:HD22	3:C:66:TYR:CD1	2.53	0.44
1:D:420:ALA:HB3	1:D:421:PRO:HD3	2.00	0.44
3:C:39:LEU:HD13	3:C:68:THR:HG22	2.00	0.44
1:A:482:VAL:HG23	4:A:606:SO4:O4	2.18	0.43
1:A:554:PHE:CD2	1:A:575:LEU:HD22	2.53	0.43
1:D:139:LEU:CD2	1:D:154:LEU:HG	2.48	0.43
2:E:106:PRO:HG3	2:E:122:LEU:HD22	2.01	0.43
2:E:60:TYR:C	2:E:60:TYR:CD1	2.92	0.43
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.54	0.43
3:C:64:LEU:HD23	3:C:65:LEU:N	2.34	0.43
2:E:127:TRP:O	2:E:138:SER:OG	2.37	0.43
2:E:71:LYS:HE3	2:E:94:LEU:HD23	2.01	0.43
2:E:167:LEU:HD23	2:E:174:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASP:OD2	1:A:110:PRO:HA	2.20	0.42
1:A:418:MET:HE3	1:A:460:LEU:HD11	2.02	0.41
1:A:322:ALA:HB1	1:A:325:VAL:HB	2.02	0.41
1:D:485:ARG:HB3	1:D:486:PRO:HD3	2.02	0.41
2:B:267:LEU:H	2:B:267:LEU:HD12	1.85	0.41
1:A:344:VAL:HG23	1:A:451:ASP:OD1	2.21	0.41
1:A:23:VAL:HG12	1:A:43:VAL:HG22	2.03	0.40
1:A:383:GLU:HB3	1:A:384:PRO:HD3	2.02	0.40
1:D:348:ARG:HG3	1:D:482:VAL:CG1	2.51	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	581/585 (99%)	572 (98%)	9 (2%)	0	100	100
1	D	575/585 (98%)	556 (97%)	16 (3%)	3 (0%)	29	41
2	B	262/274 (96%)	253 (97%)	8 (3%)	1 (0%)	34	48
2	E	262/274 (96%)	254 (97%)	7 (3%)	1 (0%)	34	48
3	C	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
3	F	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
All	All	1874/1916 (98%)	1827 (98%)	42 (2%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	113	PRO
1	D	115	LEU
2	E	102	ASN

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Mol	Chain	Res	Type
2	B	100	PRO
1	D	366	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	A	507/508 (100%)	502 (99%)	5 (1%)	76	88
1	D	503/508 (99%)	495 (98%)	8 (2%)	62	79
2	B	218/226 (96%)	215 (99%)	3 (1%)	67	82
2	E	218/226 (96%)	215 (99%)	3 (1%)	67	82
3	C	94/94 (100%)	93 (99%)	1 (1%)	73	87
3	F	94/94 (100%)	90 (96%)	4 (4%)	29	46
All	All	1634/1656 (99%)	1610 (98%)	24 (2%)	65	80

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	435	SER
1	A	460	LEU
1	A	501	GLU
1	A	570	GLU
2	B	10	HIS
2	B	187	ARG
2	B	196	LEU
3	C	70	PHE
1	D	104	GLN
1	D	138	TYR
1	D	208	GLU
1	D	232	SER
1	D	245	CYS
1	D	276	LYS
1	D	498	VAL

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Mol	Chain	Res	Type
1	D	571	GLU
2	E	5	LEU
2	E	140	ARG
2	E	143	GLN
3	F	64	LEU
3	F	70	PHE
3	F	88	SER
3	F	99	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

19 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	606	-	4,4,4	0.23	0	6,6,6	0.69	0
4	SO4	E	301	-	4,4,4	0.20	0	6,6,6	0.47	0
4	SO4	D	604	-	4,4,4	0.12	0	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	602	-	4,4,4	0.20	0	6,6,6	0.22	0
4	SO4	B	301	-	4,4,4	0.21	0	6,6,6	0.22	0
4	SO4	D	605	-	4,4,4	0.16	0	6,6,6	0.20	0
4	SO4	A	605	-	4,4,4	0.18	0	6,6,6	0.73	0
4	SO4	F	101	-	4,4,4	0.20	0	6,6,6	0.43	0
4	SO4	B	302	-	4,4,4	0.19	0	6,6,6	0.22	0
4	SO4	A	601	-	4,4,4	0.18	0	6,6,6	0.18	0
4	SO4	C	102	-	4,4,4	0.14	0	6,6,6	0.34	0
4	SO4	D	606	-	4,4,4	0.22	0	6,6,6	0.29	0
4	SO4	C	101	-	4,4,4	0.20	0	6,6,6	0.20	0
4	SO4	D	602	-	4,4,4	0.24	0	6,6,6	0.27	0
4	SO4	A	607	-	4,4,4	0.17	0	6,6,6	0.47	0
4	SO4	D	603	-	4,4,4	0.18	0	6,6,6	0.39	0
4	SO4	A	603	-	4,4,4	0.10	0	6,6,6	0.34	0
4	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.19	0
4	SO4	D	601	-	4,4,4	0.19	0	6,6,6	0.13	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	A	606	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	583/585 (99%)	-0.16	4 (0%) 87 86	27, 46, 78, 109	16 (2%)
1	D	579/585 (98%)	0.44	50 (8%) 10 9	30, 57, 107, 139	31 (5%)
2	B	264/274 (96%)	-0.13	2 (0%) 86 84	28, 42, 65, 100	7 (2%)
2	E	264/274 (96%)	-0.15	3 (1%) 80 79	28, 44, 69, 111	3 (1%)
3	C	99/99 (100%)	-0.35	0 100 100	30, 45, 71, 83	8 (8%)
3	F	99/99 (100%)	0.01	1 (1%) 82 80	35, 52, 79, 86	1 (1%)
All	All	1888/1916 (98%)	0.03	60 (3%) 47 46	27, 48, 91, 139	66 (3%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	559	CYS	5.3
1	D	370	TYR	5.2
1	D	362	ALA	5.1
1	D	302	LEU	5.1
1	D	371	ALA	4.8
1	D	310	VAL	4.8
1	D	303	PRO	3.9
1	D	568	PHE	3.8
2	E	102	ASN	3.7
1	D	516	LEU	3.7
1	A	301	ASP	3.7
1	D	118	PRO	3.6
1	D	567	CYS	3.6
1	D	364	ALA	3.5
1	D	122	VAL	3.5
1	D	111	ASN	3.5
1	A	303	PRO	3.4
1	D	275	LEU	3.4
2	E	99	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	305	LEU	3.3
1	D	300	ALA	3.3
1	D	313	LYS	3.2
1	D	116	VAL	3.1
1	D	115	LEU	3.0
1	D	556	GLU	3.0
1	D	363	ALA	2.9
1	D	542	GLU	2.8
1	D	552	ALA	2.8
1	D	555	VAL	2.8
1	D	3	HIS	2.8
1	D	369	CYS	2.7
1	D	368	GLU	2.7
1	D	376	GLU	2.7
1	D	125	THR	2.7
1	D	301	ASP	2.7
2	E	100	PRO	2.6
1	A	560	LYS	2.6
1	D	306	ALA	2.6
1	D	367	HIS	2.6
1	A	69	LEU	2.5
1	D	299	PRO	2.5
1	D	566	THR	2.5
1	D	373	VAL	2.5
1	D	171	ALA	2.5
1	D	515	THR	2.5
1	D	120	VAL	2.4
1	D	520	GLU	2.4
2	B	100	PRO	2.4
1	D	307	ALA	2.3
1	D	311	GLU	2.3
2	B	102	ASN	2.3
3	F	74	GLU	2.3
1	D	554	PHE	2.2
1	D	308	ASP	2.2
1	D	356	THR	2.2
1	D	117	ARG	2.2
1	D	372	LYS	2.1
1	D	366	PRO	2.1
1	D	374	PHE	2.0
1	D	124	CYS	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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	601	5/5	0.69	0.36	96,101,103,106	0
4	SO4	F	101	5/5	0.90	0.34	78,85,94,95	0
4	SO4	A	602	5/5	0.91	0.29	87,88,91,97	0
4	SO4	B	301	5/5	0.91	0.25	90,94,100,102	0
4	SO4	A	604	5/5	0.91	0.11	91,96,100,101	0
4	SO4	D	601	5/5	0.91	0.30	86,90,95,97	0
4	SO4	E	301	5/5	0.92	0.16	58,61,76,76	0
4	SO4	A	603	5/5	0.92	0.11	76,78,81,85	0
4	SO4	D	606	5/5	0.93	0.11	86,91,95,97	0
4	SO4	C	101	5/5	0.93	0.12	79,91,97,97	0
4	SO4	D	603	5/5	0.93	0.11	66,74,81,87	0
4	SO4	D	602	5/5	0.94	0.23	62,64,66,67	0
4	SO4	C	102	5/5	0.95	0.11	57,57,65,73	0
4	SO4	B	302	5/5	0.95	0.16	64,68,74,76	0
4	SO4	A	605	5/5	0.96	0.14	36,46,48,55	0
4	SO4	A	607	5/5	0.96	0.14	68,71,79,79	0
4	SO4	D	605	5/5	0.97	0.10	46,57,59,67	0
4	SO4	D	604	5/5	0.97	0.15	49,49,62,63	0
4	SO4	A	606	5/5	0.98	0.10	48,52,62,64	0

6.5 Other polymers (i)

There are no such residues in this entry.