Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:51 PM GMT

PDB ID	:	1MCP
Title	:	PHOSPHOCHOLINE BINDING IMMUNOGLOBULIN FAB MC/PC603. AN X-RAY DIFFRACTION STUDY AT 2.7 ANGSTROMS
Authors	:	Satow, Y.; Cohen, G.H.; Padlan, E.A.; Davies, D.R.
Deposited on	:	1984-07-09
Resolution	:	2.70 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 (i) symbol.

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

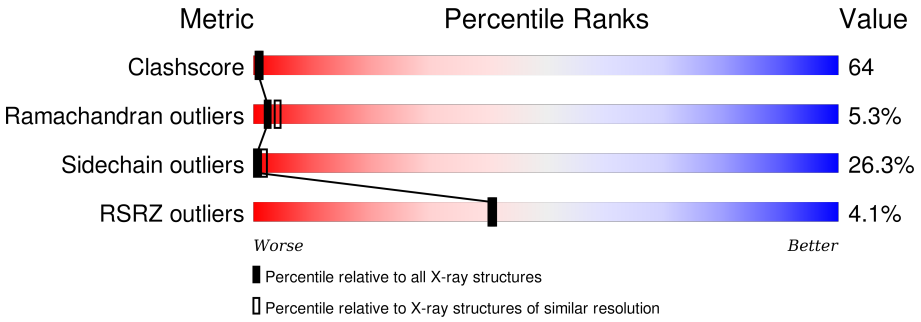
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	L	220	2% 34% 35% 25% 6%
2	H	222	3% 34% 41% 15% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3544 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 IGA-KAPPA MCPC603 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	220	1692	1048	286	350	8	0	0	0

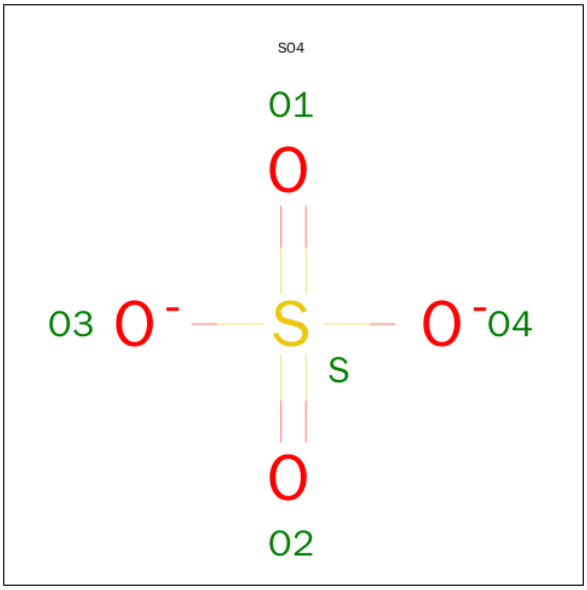
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	112	ILE	LEU	CONFLICT	GB 208622

- Molecule 2 is a protein called IGA-KAPPA MCPC603 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	222	1709	1079	286	334	10	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

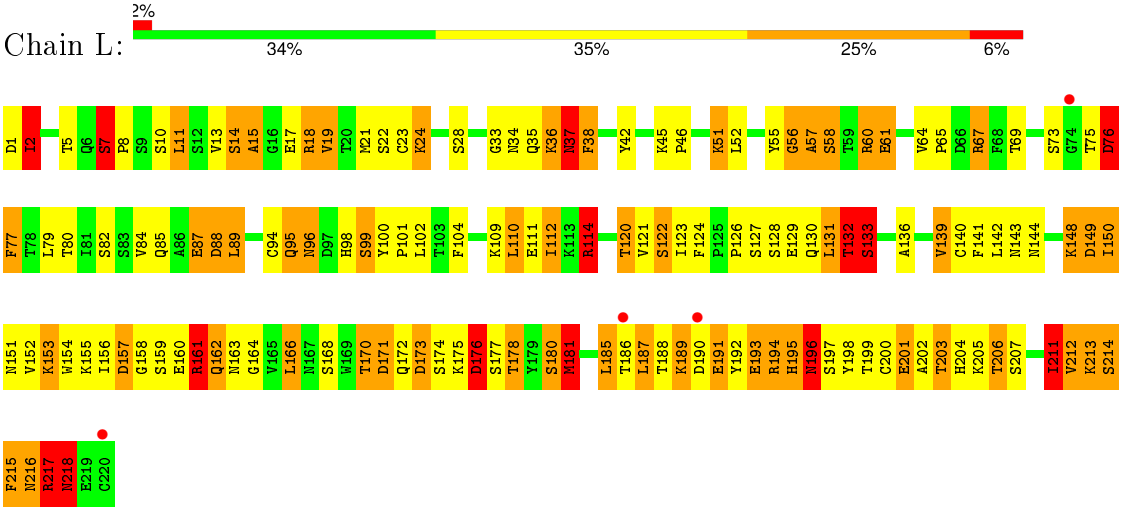
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	76	Total O 76 76	0	0
4	L	62	Total O 62 62	0	0

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.

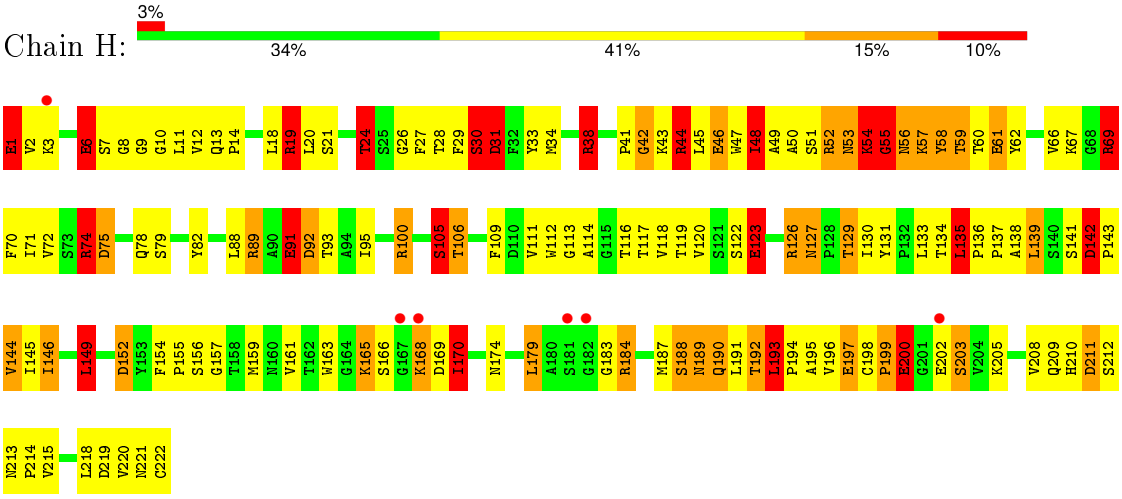
- Molecule 1: IGA-KAPPA MCPC603 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: IGA-KAPPA MCPC603 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	162.53Å 162.53Å 60.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70 7.99 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70) 96.5 (7.99-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.225 , (Not available) 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 83.0	EDS
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 23737 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3544	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]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: 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	L	1.16	3/1728 (0.2%)	2.16	56/2344 (2.4%)
2	H	1.20	4/1753 (0.2%)	2.16	63/2389 (2.6%)
All	All	1.18	7/3481 (0.2%)	2.16	119/4733 (2.5%)

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	L	0	3
2	H	0	5
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	42	GLY	N-CA	7.02	1.56	1.46
2	H	105	SER	CB-OG	6.62	1.50	1.42
2	H	6	GLU	CG-CD	-6.00	1.43	1.51
1	L	56	GLY	N-CA	5.62	1.54	1.46
1	L	114	ARG	CD-NE	-5.50	1.37	1.46
2	H	55	GLY	N-CA	5.38	1.54	1.46
1	L	10	SER	CB-OG	5.26	1.49	1.42

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	114	ARG	NE-CZ-NH1	29.10	134.85	120.30
1	L	114	ARG	CD-NE-CZ	19.61	151.05	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	126	ARG	NE-CZ-NH2	-19.02	110.79	120.30
2	H	100	ARG	CD-NE-CZ	17.89	148.64	123.60
1	L	60	ARG	NE-CZ-NH2	17.66	129.13	120.30
2	H	126	ARG	NE-CZ-NH1	16.12	128.36	120.30
2	H	19	ARG	NE-CZ-NH1	15.72	128.16	120.30
2	H	100	ARG	NE-CZ-NH1	14.99	127.79	120.30
1	L	176	ASP	CB-CG-OD1	-13.35	106.29	118.30
2	H	100	ARG	NE-CZ-NH2	-12.83	113.89	120.30
2	H	126	ARG	CD-NE-CZ	-12.70	105.83	123.60
1	L	60	ARG	CD-NE-CZ	12.59	141.23	123.60
2	H	92	ASP	CB-CG-OD2	12.17	129.25	118.30
2	H	126	ARG	CG-CD-NE	11.68	136.32	111.80
1	L	109	LYS	CA-CB-CG	10.95	137.50	113.40
2	H	74	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	L	185	LEU	CA-CB-CG	10.47	139.38	115.30
1	L	76	ASP	CB-CG-OD1	9.96	127.27	118.30
2	H	38	ARG	NE-CZ-NH2	-9.82	115.39	120.30
2	H	89	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	H	1	GLU	OE1-CD-OE2	9.47	134.66	123.30
2	H	89	ARG	CD-NE-CZ	9.39	136.75	123.60
1	L	166	LEU	CA-CB-CG	9.20	136.45	115.30
1	L	114	ARG	NH1-CZ-NH2	-9.15	109.33	119.40
2	H	44	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	L	114	ARG	NE-CZ-NH2	-8.97	115.81	120.30
2	H	31	ASP	CB-CG-OD1	-8.88	110.31	118.30
1	L	87	GLU	OE1-CD-OE2	8.57	133.58	123.30
1	L	88	ASP	CB-CG-OD1	8.47	125.92	118.30
1	L	2	ILE	CB-CA-C	8.45	128.50	111.60
1	L	211	ILE	CB-CA-C	8.40	128.39	111.60
2	H	19	ARG	NH1-CZ-NH2	-8.39	110.17	119.40
1	L	18	ARG	NE-CZ-NH2	-8.38	116.11	120.30
2	H	184	ARG	CD-NE-CZ	-8.26	112.04	123.60
2	H	6	GLU	CG-CD-OE1	8.15	134.61	118.30
2	H	82	TYR	CB-CG-CD1	-8.12	116.13	121.00
2	H	100	ARG	CA-CB-CG	8.10	131.22	113.40
1	L	60	ARG	NH1-CZ-NH2	-7.94	110.67	119.40
1	L	213	LYS	N-CA-CB	7.89	124.80	110.60
1	L	217	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	H	19	ARG	CD-NE-CZ	7.78	134.49	123.60
1	L	56	GLY	N-CA-C	-7.68	93.91	113.10
2	H	211	ASP	CB-CG-OD1	7.66	125.19	118.30
1	L	173	ASP	CB-CG-OD1	7.58	125.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	67	ARG	NE-CZ-NH2	-7.28	116.66	120.30
2	H	189	ASN	N-CA-CB	-7.26	97.53	110.60
1	L	157	ASP	CA-CB-CG	7.19	129.22	113.40
1	L	2	ILE	CA-CB-CG1	6.96	124.23	111.00
2	H	61	GLU	CA-CB-CG	6.89	128.56	113.40
1	L	194	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	L	56	GLY	CA-C-O	-6.79	108.37	120.60
2	H	44	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	H	82	TYR	CB-CG-CD2	6.74	125.05	121.00
1	L	57	ALA	CB-CA-C	6.69	120.14	110.10
1	L	37	ASN	CA-CB-CG	6.66	128.06	113.40
2	H	184	ARG	NE-CZ-NH1	-6.64	116.98	120.30
2	H	149	LEU	CB-CA-C	6.54	122.62	110.20
2	H	48	ILE	CA-C-N	6.51	131.53	117.20
2	H	56	ASN	OD1-CG-ND2	6.51	136.88	121.90
2	H	200	GLU	OE1-CD-OE2	6.44	131.02	123.30
1	L	173	ASP	CB-CG-OD2	-6.40	112.54	118.30
2	H	74	ARG	NH1-CZ-NH2	-6.34	112.42	119.40
1	L	191	GLU	CB-CG-CD	6.34	131.31	114.20
2	H	74	ARG	CA-CB-CG	6.33	127.33	113.40
2	H	135	LEU	CA-CB-CG	6.33	129.86	115.30
2	H	34	MET	CB-CA-C	6.28	122.96	110.40
1	L	196	ASN	CA-CB-CG	-6.22	99.71	113.40
1	L	61	GLU	CG-CD-OE1	6.20	130.69	118.30
2	H	56	ASN	CB-CG-OD1	-6.20	109.21	121.60
1	L	191	GLU	CG-CD-OE1	6.12	130.54	118.30
1	L	24	LYS	CA-CB-CG	6.10	126.82	113.40
1	L	187	LEU	CB-CA-C	6.00	121.61	110.20
2	H	193	LEU	CA-CB-CG	5.99	129.07	115.30
2	H	46	GLU	CG-CD-OE2	-5.91	106.48	118.30
2	H	69	ARG	CD-NE-CZ	-5.91	115.33	123.60
2	H	152	ASP	CB-CG-OD1	5.88	123.60	118.30
1	L	141	PHE	CA-CB-CG	5.88	128.01	113.90
2	H	6	GLU	CB-CG-CD	5.81	129.89	114.20
1	L	94	CYS	O-C-N	5.76	131.91	122.70
1	L	181	MET	CG-SD-CE	5.75	109.40	100.20
2	H	127	ASN	CA-CB-CG	5.74	126.02	113.40
1	L	212	VAL	N-CA-CB	-5.73	98.90	111.50
2	H	91	GLU	CA-CB-CG	5.72	125.98	113.40
2	H	156	SER	N-CA-CB	5.71	119.06	110.50
2	H	24	THR	N-CA-CB	-5.61	99.64	110.30
2	H	219	ASP	CB-CG-OD2	-5.60	113.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	180	SER	N-CA-CB	5.60	118.89	110.50
2	H	48	ILE	O-C-N	-5.49	113.92	122.70
2	H	54	LYS	CA-C-O	-5.48	108.60	120.10
1	L	15	ALA	CB-CA-C	-5.47	101.90	110.10
1	L	18	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	L	176	ASP	CA-CB-CG	-5.45	101.41	113.40
1	L	58	SER	N-CA-C	5.39	125.55	111.00
1	L	176	ASP	OD1-CG-OD2	5.38	133.51	123.30
2	H	56	ASN	CB-CA-C	5.35	121.10	110.40
1	L	7	SER	N-CA-CB	-5.34	102.50	110.50
1	L	194	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	H	146	ILE	CA-CB-CG1	5.30	121.07	111.00
2	H	123	GLU	OE1-CD-OE2	5.29	129.65	123.30
2	H	41	PRO	CA-C-N	5.29	126.77	116.20
2	H	105	SER	N-CA-CB	-5.25	102.62	110.50
2	H	6	GLU	OE1-CD-OE2	-5.24	117.01	123.30
2	H	54	LYS	CB-CA-C	-5.24	99.93	110.40
1	L	218	ASN	CB-CA-C	5.23	120.86	110.40
1	L	159	SER	N-CA-C	-5.22	96.91	111.00
2	H	52	ARG	CD-NE-CZ	5.21	130.90	123.60
1	L	191	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	L	149	ASP	CB-CG-OD1	5.21	122.99	118.30
1	L	131	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	L	132	THR	CB-CA-C	5.18	125.59	111.60
1	L	14	SER	N-CA-CB	5.13	118.20	110.50
2	H	170	ILE	O-C-N	5.11	130.87	122.70
2	H	33	TYR	O-C-N	5.09	130.85	122.70
1	L	77	PHE	O-C-N	5.08	130.82	122.70
2	H	219	ASP	O-C-N	5.07	130.81	122.70
2	H	149	LEU	CA-CB-CG	5.04	126.88	115.30
2	H	156	SER	CB-CA-C	5.03	119.66	110.10
1	L	162	GLN	N-CA-CB	-5.02	101.56	110.60
2	H	55	GLY	N-CA-C	-5.01	100.57	113.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	126	ARG	Sidechain
2	H	129	THR	Mainchain
2	H	19	ARG	Sidechain
2	H	44	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	H	54	LYS	Mainchain
1	L	161	ARG	Sidechain
1	L	2	ILE	Mainchain
1	L	217	ARG	Sidechain

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	L	1692	0	1622	231	14
2	H	1709	0	1648	207	13
3	H	5	0	0	1	0
4	H	76	0	0	8	1
4	L	62	0	0	14	0
All	All	3544	0	3270	428	15

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 64.

All (428) 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:L:153:LYS:NZ	1:L:161:ARG:HD3	1.37	1.36
1:L:34:ASN:CB	1:L:36:LYS:HE3	1.72	1.19
2:H:169:ASP:O	2:H:170:ILE:HG13	1.42	1.17
1:L:160:GLU:O	1:L:161:ARG:HG3	1.44	1.16
1:L:201:GLU:CB	1:L:212:VAL:HG22	1.77	1.13
1:L:14:SER:O	1:L:15:ALA:HB3	1.48	1.12
2:H:49:ALA:CB	2:H:72:VAL:HG21	1.80	1.12
2:H:169:ASP:CG	2:H:194:PRO:HD3	1.72	1.09
1:L:34:ASN:HB3	1:L:36:LYS:CE	1.81	1.08
2:H:136:PRO:HG2	2:H:139:LEU:HG	1.28	1.08
1:L:199:THR:HG22	1:L:214:SER:HB2	1.28	1.08
2:H:131:TYR:HB2	2:H:149:LEU:CD1	1.85	1.06
1:L:153:LYS:NZ	1:L:161:ARG:CD	2.19	1.05
1:L:153:LYS:CD	1:L:161:ARG:HG2	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:ALA:HB1	2:H:72:VAL:CG2	1.86	1.04
1:L:201:GLU:HB2	1:L:212:VAL:HG22	1.39	1.03
2:H:8:GLY:O	2:H:20:LEU:CD2	2.07	1.03
1:L:195:HIS:O	1:L:218:ASN:ND2	1.93	1.01
1:L:157:ASP:CG	1:L:195:HIS:HB3	1.78	1.00
1:L:153:LYS:HZ2	1:L:161:ARG:HD3	0.93	1.00
1:L:34:ASN:HB2	1:L:36:LYS:HE3	1.41	1.00
1:L:14:SER:O	1:L:15:ALA:CB	2.09	0.99
2:H:24:THR:HG22	2:H:24:THR:O	1.60	0.99
2:H:49:ALA:HB1	2:H:72:VAL:HG21	1.01	0.98
1:L:216:ASN:O	1:L:217:ARG:CG	2.12	0.98
2:H:11:LEU:HD13	2:H:155:PRO:HG3	1.45	0.97
2:H:138:ALA:O	2:H:139:LEU:HD23	1.64	0.96
1:L:34:ASN:CB	1:L:36:LYS:CE	2.42	0.96
2:H:49:ALA:CB	2:H:72:VAL:CG2	2.44	0.95
2:H:169:ASP:OD2	2:H:194:PRO:HD3	1.65	0.95
1:L:152:VAL:HG21	1:L:181:MET:HE2	1.47	0.94
1:L:152:VAL:HG21	1:L:181:MET:CE	1.98	0.94
2:H:138:ALA:C	2:H:139:LEU:HD23	1.89	0.93
2:H:52:ARG:HE	2:H:59:THR:HG22	1.31	0.92
1:L:188:THR:OG1	1:L:191:GLU:HB2	1.67	0.92
1:L:191:GLU:HA	1:L:194:ARG:HD2	1.47	0.92
1:L:153:LYS:HZ3	1:L:161:ARG:CG	1.83	0.92
1:L:153:LYS:HZ3	1:L:161:ARG:HD3	1.31	0.90
2:H:136:PRO:HG2	2:H:139:LEU:CG	1.99	0.90
1:L:201:GLU:HB3	1:L:212:VAL:HG22	1.52	0.90
1:L:153:LYS:HZ3	1:L:161:ARG:CD	1.82	0.90
2:H:136:PRO:HD2	2:H:139:LEU:HD12	1.54	0.90
1:L:190:ASP:HA	4:L:346:HOH:O	1.71	0.89
1:L:96:ASN:ND2	1:L:98:HIS:H	1.71	0.89
2:H:54:LYS:HB2	2:H:58:TYR:OH	1.72	0.89
1:L:34:ASN:HB3	1:L:36:LYS:HE2	1.53	0.88
1:L:1:ASP:HB3	4:L:226:HOH:O	1.73	0.88
1:L:198:TYR:HB2	1:L:215:PHE:CE2	2.10	0.87
2:H:131:TYR:HB2	2:H:149:LEU:HD11	1.55	0.86
2:H:169:ASP:C	2:H:169:ASP:OD1	2.13	0.86
1:L:216:ASN:O	1:L:217:ARG:HG2	1.73	0.86
1:L:67:ARG:NH1	1:L:88:ASP:OD2	2.09	0.86
1:L:212:VAL:O	1:L:212:VAL:HG12	1.75	0.86
2:H:202:GLU:O	2:H:203:SER:HB3	1.73	0.86
1:L:37:ASN:HD22	1:L:57:ALA:HB2	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:GLU:HG3	4:H:305:HOH:O	1.74	0.85
2:H:169:ASP:OD2	2:H:194:PRO:CD	2.24	0.85
1:L:160:GLU:O	1:L:161:ARG:CG	2.24	0.84
2:H:105:SER:HB2	2:H:106:THR:HG22	1.58	0.84
1:L:176:ASP:N	1:L:176:ASP:OD1	2.05	0.84
2:H:54:LYS:O	2:H:54:LYS:CG	2.18	0.84
2:H:66:VAL:HG13	2:H:70:PHE:HB2	1.60	0.83
2:H:93:THR:HG23	2:H:119:THR:HA	1.61	0.83
1:L:151:ASN:OD1	1:L:203:THR:HG22	1.79	0.82
2:H:142:ASP:OD1	2:H:142:ASP:C	2.18	0.81
1:L:1:ASP:CB	4:L:226:HOH:O	2.25	0.81
1:L:153:LYS:HD2	1:L:161:ARG:HG2	1.61	0.81
1:L:42:TYR:OH	1:L:95:GLN:NE2	2.13	0.81
1:L:128:SER:O	1:L:132:THR:HG23	1.80	0.80
1:L:153:LYS:HD2	1:L:161:ARG:NE	1.97	0.80
1:L:150:ILE:HG23	1:L:150:ILE:O	1.81	0.80
1:L:196:ASN:N	1:L:196:ASN:HD22	1.80	0.79
2:H:62:TYR:HE1	2:H:72:VAL:HG23	1.47	0.79
2:H:38:ARG:NH2	2:H:46:GLU:OE2	2.15	0.79
1:L:153:LYS:HD2	1:L:161:ARG:CG	2.12	0.79
1:L:217:ARG:O	1:L:218:ASN:CB	2.30	0.79
1:L:24:LYS:HD3	1:L:76:ASP:OD1	1.83	0.78
1:L:173:ASP:OD2	1:L:173:ASP:C	2.21	0.78
2:H:131:TYR:HB2	2:H:149:LEU:HD13	1.65	0.78
1:L:153:LYS:HD2	1:L:161:ARG:CD	2.14	0.77
1:L:188:THR:OG1	1:L:191:GLU:CB	2.30	0.77
1:L:202:ALA:N	1:L:211:ILE:O	2.16	0.77
2:H:196:VAL:O	2:H:196:VAL:HG22	1.83	0.77
2:H:161:VAL:HG11	2:H:189:ASN:ND2	1.99	0.76
1:L:201:GLU:HA	1:L:211:ILE:O	1.86	0.76
2:H:202:GLU:O	2:H:203:SER:CB	2.33	0.76
1:L:42:TYR:CE1	1:L:95:GLN:NE2	2.54	0.76
1:L:157:ASP:CB	1:L:195:HIS:HB3	2.15	0.75
2:H:53:ASN:O	2:H:55:GLY:N	2.19	0.75
2:H:145:ILE:CG2	2:H:190:GLN:HE21	1.99	0.74
2:H:54:LYS:O	2:H:54:LYS:CD	2.35	0.74
1:L:170:THR:HG23	1:L:171:ASP:O	1.88	0.74
1:L:216:ASN:O	1:L:217:ARG:HG3	1.84	0.74
1:L:18:ARG:O	4:L:349:HOH:O	2.04	0.74
2:H:42:GLY:O	2:H:43:LYS:HG2	1.88	0.73
2:H:52:ARG:NE	2:H:59:THR:HG22	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:VAL:CG1	2:H:189:ASN:ND2	2.52	0.73
2:H:6:GLU:HA	2:H:21:SER:O	1.89	0.73
1:L:11:LEU:CD2	1:L:19:VAL:CG2	2.66	0.73
1:L:197:SER:HA	1:L:216:ASN:HB3	1.70	0.73
1:L:42:TYR:HE1	1:L:95:GLN:HE21	1.35	0.73
2:H:136:PRO:O	2:H:138:ALA:N	2.23	0.72
2:H:24:THR:CG2	2:H:24:THR:O	2.30	0.72
1:L:173:ASP:OD2	1:L:174:SER:N	2.22	0.72
2:H:62:TYR:CE1	2:H:72:VAL:HG23	2.25	0.72
1:L:96:ASN:HD22	1:L:98:HIS:H	1.36	0.72
1:L:216:ASN:C	1:L:217:ARG:HG3	2.10	0.72
2:H:1:GLU:O	2:H:26:GLY:HA3	1.90	0.72
2:H:117:THR:HG21	2:H:157:GLY:HA2	1.71	0.71
1:L:153:LYS:HD3	1:L:161:ARG:HG2	1.73	0.71
2:H:136:PRO:HD2	2:H:139:LEU:CD1	2.19	0.71
1:L:114:ARG:HD2	1:L:176:ASP:O	1.90	0.71
2:H:105:SER:CB	2:H:106:THR:HG22	2.20	0.71
1:L:17:GLU:OE2	4:L:301:HOH:O	2.08	0.71
1:L:195:HIS:CD2	1:L:195:HIS:H	2.08	0.71
1:L:153:LYS:HD2	1:L:161:ARG:HE	1.55	0.71
2:H:123:GLU:O	4:H:310:HOH:O	2.07	0.71
2:H:145:ILE:CD1	2:H:192:THR:HB	2.21	0.71
1:L:187:LEU:HD11	1:L:192:TYR:HB2	1.73	0.70
2:H:31:ASP:HA	2:H:53:ASN:HB2	1.73	0.70
1:L:198:TYR:CB	1:L:215:PHE:CE2	2.75	0.70
2:H:54:LYS:HB2	2:H:58:TYR:CZ	2.27	0.69
2:H:169:ASP:CG	2:H:194:PRO:CD	2.58	0.69
1:L:151:ASN:OD1	1:L:203:THR:CG2	2.40	0.69
1:L:156:ILE:HG23	1:L:198:TYR:CE1	2.27	0.69
2:H:75:ASP:OD2	2:H:78:GLN:HB2	1.93	0.69
1:L:187:LEU:CD1	1:L:192:TYR:HB2	2.23	0.69
1:L:201:GLU:HB2	1:L:212:VAL:CG2	2.19	0.68
1:L:173:ASP:OD2	1:L:175:LYS:N	2.26	0.68
2:H:10:GLY:HA3	4:H:275:HOH:O	1.92	0.68
2:H:163:TRP:HE1	2:H:189:ASN:ND2	1.92	0.68
2:H:169:ASP:OD1	2:H:170:ILE:N	2.26	0.68
1:L:157:ASP:OD1	1:L:195:HIS:HB3	1.91	0.68
1:L:114:ARG:HD2	1:L:177:SER:HB2	1.74	0.68
1:L:11:LEU:CD2	1:L:19:VAL:HG22	2.23	0.68
2:H:145:ILE:HD12	2:H:192:THR:HB	1.76	0.68
2:H:145:ILE:HG23	2:H:190:GLN:HE21	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:SER:O	2:H:31:ASP:HB3	1.92	0.68
1:L:37:ASN:HD21	1:L:73:SER:HA	1.58	0.67
1:L:11:LEU:HD21	1:L:19:VAL:HG22	1.76	0.67
2:H:88:LEU:HB3	2:H:120:VAL:HG21	1.76	0.67
1:L:162:GLN:HG3	1:L:163:ASN:H	1.59	0.67
2:H:24:THR:HG21	2:H:29:PHE:CD1	2.30	0.67
2:H:136:PRO:CG	2:H:139:LEU:CD1	2.73	0.67
1:L:172:GLN:HG2	1:L:177:SER:HA	1.77	0.66
2:H:145:ILE:CG2	2:H:190:GLN:NE2	2.58	0.66
2:H:89:ARG:HE	2:H:91:GLU:CD	1.98	0.66
2:H:170:ILE:HG12	2:H:193:LEU:HB2	1.76	0.66
2:H:29:PHE:CE2	2:H:74:ARG:HD3	2.30	0.66
1:L:176:ASP:OD2	1:L:178:THR:OG1	2.14	0.66
2:H:6:GLU:OE2	2:H:113:GLY:HA3	1.95	0.66
1:L:131:LEU:O	1:L:133:SER:N	2.19	0.66
1:L:34:ASN:HD22	1:L:36:LYS:NZ	1.93	0.66
1:L:124:PHE:CD1	2:H:135:LEU:HG	2.31	0.66
2:H:44:ARG:HG3	2:H:45:LEU:O	1.96	0.66
2:H:159:MET:SD	2:H:208:VAL:HG12	2.36	0.66
2:H:31:ASP:HA	2:H:53:ASN:CB	2.25	0.65
2:H:48:ILE:HG13	2:H:49:ALA:H	1.62	0.65
1:L:131:LEU:HD21	1:L:136:ALA:HB2	1.78	0.65
1:L:120:THR:HG22	4:L:344:HOH:O	1.97	0.65
1:L:11:LEU:HD22	1:L:19:VAL:HG21	1.78	0.65
1:L:153:LYS:HZ3	1:L:161:ARG:CB	2.10	0.65
2:H:136:PRO:CG	2:H:139:LEU:HD11	2.27	0.65
2:H:8:GLY:O	2:H:20:LEU:HD22	1.95	0.65
1:L:155:LYS:HG2	1:L:160:GLU:H	1.61	0.65
1:L:156:ILE:O	1:L:197:SER:O	2.15	0.65
1:L:153:LYS:NZ	1:L:161:ARG:CG	2.54	0.64
1:L:37:ASN:ND2	1:L:77:PHE:HE2	1.94	0.64
1:L:162:GLN:CG	1:L:163:ASN:N	2.59	0.64
1:L:42:TYR:CZ	1:L:95:GLN:NE2	2.65	0.64
1:L:55:TYR:C	1:L:56:GLY:O	2.29	0.64
1:L:201:GLU:CB	1:L:212:VAL:CG2	2.67	0.64
2:H:8:GLY:O	2:H:20:LEU:HD23	1.96	0.64
2:H:159:MET:SD	2:H:208:VAL:CG1	2.87	0.63
2:H:161:VAL:HG11	2:H:189:ASN:HD22	1.63	0.63
2:H:136:PRO:CG	2:H:139:LEU:HG	2.18	0.63
1:L:67:ARG:HH12	1:L:88:ASP:CG	2.02	0.63
2:H:163:TRP:NE1	2:H:189:ASN:ND2	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:ASN:ND2	1:L:73:SER:HA	2.13	0.63
1:L:131:LEU:C	1:L:133:SER:H	2.02	0.63
1:L:11:LEU:CD2	1:L:19:VAL:HG21	2.29	0.63
2:H:50:ALA:O	2:H:60:THR:HA	1.98	0.63
1:L:216:ASN:C	1:L:217:ARG:CG	2.65	0.62
1:L:162:GLN:CG	1:L:163:ASN:H	2.11	0.62
1:L:201:GLU:CA	1:L:211:ILE:O	2.47	0.62
1:L:217:ARG:O	1:L:218:ASN:HB3	1.98	0.62
1:L:89:LEU:HD23	1:L:110:LEU:O	1.99	0.62
2:H:8:GLY:O	2:H:20:LEU:HD21	2.00	0.62
2:H:56:ASN:C	2:H:57:LYS:HG2	2.18	0.62
2:H:142:ASP:OD1	2:H:143:PRO:N	2.33	0.62
2:H:9:GLY:O	2:H:212:SER:HB3	2.00	0.61
1:L:51:LYS:HG3	1:L:51:LYS:O	1.99	0.61
1:L:212:VAL:O	1:L:212:VAL:CG1	2.43	0.61
1:L:162:GLN:HG2	1:L:164:GLY:H	1.66	0.61
2:H:54:LYS:HG2	2:H:54:LYS:O	1.94	0.60
1:L:196:ASN:N	1:L:196:ASN:ND2	2.49	0.60
2:H:136:PRO:CG	2:H:139:LEU:CG	2.79	0.60
2:H:56:ASN:O	2:H:57:LYS:O	2.18	0.60
1:L:121:VAL:HG12	1:L:122:SER:N	2.16	0.60
1:L:176:ASP:O	1:L:177:SER:HB2	2.01	0.60
2:H:66:VAL:CG1	2:H:70:PHE:HB2	2.32	0.60
1:L:142:LEU:HD13	1:L:181:MET:HG2	1.84	0.60
1:L:198:TYR:N	1:L:215:PHE:O	2.24	0.59
2:H:66:VAL:HG13	2:H:70:PHE:CB	2.30	0.59
1:L:197:SER:HA	1:L:216:ASN:HA	1.83	0.59
2:H:52:ARG:NH1	3:H:223:SO4:O3	2.36	0.59
2:H:7:SER:HB2	4:H:279:HOH:O	2.03	0.59
1:L:186:THR:HG23	1:L:186:THR:O	2.03	0.59
2:H:19:ARG:NE	4:H:293:HOH:O	2.35	0.59
1:L:153:LYS:CE	1:L:161:ARG:HG2	2.33	0.59
1:L:153:LYS:HZ2	1:L:161:ARG:CD	1.88	0.59
2:H:136:PRO:CD	2:H:139:LEU:CD1	2.81	0.58
1:L:157:ASP:HB2	1:L:195:HIS:HB3	1.83	0.58
1:L:42:TYR:HE1	1:L:95:GLN:NE2	1.96	0.58
2:H:169:ASP:O	2:H:170:ILE:CG1	2.34	0.58
1:L:218:ASN:OD1	1:L:218:ASN:C	2.38	0.58
1:L:150:ILE:O	1:L:150:ILE:CG2	2.50	0.58
1:L:204:HIS:ND1	1:L:206:THR:OG1	2.34	0.58
1:L:153:LYS:CD	1:L:161:ARG:CG	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:196:ASN:O	1:L:216:ASN:HA	2.04	0.57
1:L:168:SER:O	1:L:181:MET:HA	2.04	0.57
2:H:52:ARG:NH2	2:H:59:THR:CG2	2.68	0.57
2:H:53:ASN:C	2:H:55:GLY:N	2.56	0.57
2:H:169:ASP:OD2	2:H:194:PRO:HG3	2.05	0.57
2:H:29:PHE:CZ	2:H:74:ARG:HD3	2.41	0.56
2:H:66:VAL:HG13	2:H:70:PHE:CG	2.40	0.56
1:L:157:ASP:HB2	1:L:195:HIS:CB	2.35	0.56
1:L:217:ARG:O	1:L:218:ASN:HB2	2.06	0.56
1:L:11:LEU:HD22	1:L:19:VAL:CG2	2.33	0.56
2:H:69:ARG:NH2	2:H:92:ASP:OD1	2.38	0.56
1:L:189:LYS:HD3	4:L:306:HOH:O	2.05	0.56
1:L:101:PRO:HB3	2:H:47:TRP:CZ3	2.41	0.56
2:H:169:ASP:OD2	2:H:194:PRO:CG	2.53	0.56
1:L:201:GLU:HB3	1:L:212:VAL:CG2	2.30	0.56
2:H:145:ILE:HG21	2:H:190:GLN:NE2	2.20	0.56
2:H:136:PRO:O	2:H:139:LEU:HG	2.06	0.56
2:H:52:ARG:NE	2:H:59:THR:CG2	2.69	0.56
2:H:130:ILE:HD12	2:H:208:VAL:HG21	1.86	0.55
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.89	0.55
1:L:196:ASN:H	1:L:196:ASN:HD22	1.55	0.55
1:L:126:PRO:HG2	1:L:192:TYR:CZ	2.41	0.55
1:L:131:LEU:CD2	1:L:136:ALA:HB2	2.37	0.55
1:L:149:ASP:O	4:L:327:HOH:O	2.17	0.55
1:L:200:CYS:O	1:L:212:VAL:HA	2.06	0.55
1:L:152:VAL:CG2	1:L:181:MET:CE	2.79	0.55
2:H:52:ARG:HH21	2:H:59:THR:CG2	2.20	0.55
2:H:56:ASN:C	2:H:56:ASN:OD1	2.44	0.55
1:L:37:ASN:HD22	1:L:57:ALA:CB	2.18	0.55
1:L:187:LEU:HD11	1:L:192:TYR:CB	2.35	0.54
2:H:42:GLY:HA3	4:H:253:HOH:O	2.06	0.54
1:L:121:VAL:CG1	1:L:122:SER:N	2.71	0.54
2:H:56:ASN:C	2:H:57:LYS:CG	2.75	0.54
2:H:28:THR:HG22	2:H:28:THR:O	2.06	0.54
2:H:24:THR:HG21	2:H:29:PHE:HB2	1.90	0.54
2:H:19:ARG:CD	4:H:293:HOH:O	2.55	0.54
2:H:145:ILE:HD13	2:H:192:THR:HB	1.90	0.54
1:L:196:ASN:O	1:L:217:ARG:N	2.38	0.54
1:L:153:LYS:HZ3	1:L:161:ARG:HB3	1.73	0.53
2:H:130:ILE:HG22	2:H:218:LEU:HD22	1.90	0.53
2:H:163:TRP:HE1	2:H:189:ASN:HD21	1.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:145:ILE:HG23	2:H:190:GLN:NE2	2.23	0.53
1:L:198:TYR:HB2	1:L:215:PHE:CD2	2.42	0.53
2:H:53:ASN:C	2:H:53:ASN:HD22	2.08	0.53
1:L:110:LEU:CD1	1:L:112:ILE:HD13	2.39	0.52
2:H:142:ASP:HA	2:H:143:PRO:C	2.30	0.52
1:L:152:VAL:CG2	1:L:181:MET:HE1	2.39	0.52
2:H:161:VAL:HG12	2:H:189:ASN:ND2	2.24	0.52
1:L:124:PHE:CE1	2:H:135:LEU:HG	2.43	0.52
2:H:165:LYS:NZ	2:H:197:GLU:O	2.41	0.52
1:L:193:GLU:HA	1:L:218:ASN:OD1	2.09	0.52
1:L:96:ASN:C	1:L:96:ASN:ND2	2.64	0.52
2:H:24:THR:HG23	2:H:27:PHE:CZ	2.45	0.51
2:H:31:ASP:C	2:H:31:ASP:OD1	2.49	0.51
1:L:127:SER:O	1:L:131:LEU:HG	2.10	0.51
1:L:161:ARG:O	1:L:162:GLN:HB2	2.09	0.51
1:L:36:LYS:NZ	2:H:105:SER:O	2.36	0.51
2:H:198:CYS:N	2:H:199:PRO:CD	2.73	0.51
2:H:2:VAL:HG12	2:H:111:VAL:HG21	1.93	0.51
1:L:101:PRO:HB3	2:H:47:TRP:HZ3	1.76	0.51
1:L:156:ILE:O	1:L:198:TYR:HA	2.10	0.51
1:L:101:PRO:CB	2:H:47:TRP:CZ3	2.94	0.51
2:H:161:VAL:HG21	2:H:187:MET:CE	2.40	0.51
2:H:135:LEU:HB3	2:H:139:LEU:HB2	1.92	0.51
2:H:75:ASP:OD1	2:H:75:ASP:C	2.50	0.51
2:H:144:VAL:CG2	2:H:195:ALA:HA	2.41	0.50
1:L:24:LYS:HA	1:L:75:THR:O	2.10	0.50
2:H:42:GLY:C	2:H:43:LYS:CG	2.80	0.50
2:H:42:GLY:O	2:H:43:LYS:CG	2.59	0.50
1:L:1:ASP:OD1	1:L:101:PRO:HG3	2.11	0.50
1:L:139:VAL:CG1	2:H:133:LEU:HD21	2.42	0.50
2:H:179:LEU:HD21	2:H:183:GLY:C	2.32	0.50
2:H:202:GLU:OE1	2:H:202:GLU:HA	2.12	0.50
2:H:152:ASP:OD2	2:H:184:ARG:NH1	2.44	0.50
1:L:38:PHE:CD1	1:L:38:PHE:N	2.79	0.50
2:H:169:ASP:O	2:H:169:ASP:CG	2.49	0.49
2:H:136:PRO:HG3	2:H:139:LEU:HD11	1.93	0.49
2:H:69:ARG:HH22	2:H:92:ASP:CG	2.14	0.49
1:L:197:SER:CA	1:L:216:ASN:HB3	2.41	0.49
2:H:144:VAL:O	2:H:145:ILE:HD13	2.12	0.49
2:H:213:ASN:HB3	2:H:214:PRO:HD2	1.94	0.49
1:L:37:ASN:ND2	1:L:57:ALA:HB2	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:134:THR:HG21	2:H:221:ASN:O	2.12	0.49
1:L:216:ASN:ND2	4:L:295:HOH:O	2.46	0.49
1:L:96:ASN:ND2	1:L:98:HIS:N	2.52	0.49
2:H:141:SER:O	2:H:142:ASP:HB3	2.13	0.49
1:L:77:PHE:HB3	4:L:313:HOH:O	2.12	0.49
1:L:114:ARG:CD	1:L:177:SER:HB2	2.42	0.49
1:L:196:ASN:ND2	1:L:197:SER:N	2.61	0.48
2:H:24:THR:HG21	2:H:29:PHE:HD1	1.78	0.48
2:H:163:TRP:CE3	2:H:191:LEU:HD22	2.48	0.48
2:H:31:ASP:CA	2:H:53:ASN:HB2	2.42	0.48
2:H:11:LEU:HD11	2:H:154:PHE:HE2	1.77	0.48
1:L:112:ILE:H	1:L:172:GLN:HE22	1.60	0.48
1:L:34:ASN:O	1:L:35:GLN:HB2	2.13	0.48
1:L:89:LEU:HD11	1:L:172:GLN:HB3	1.95	0.48
1:L:110:LEU:HD11	1:L:112:ILE:HD13	1.95	0.48
1:L:130:GLN:HB2	2:H:131:TYR:CE2	2.49	0.48
2:H:52:ARG:NH2	2:H:59:THR:HG21	2.28	0.48
2:H:31:ASP:C	2:H:53:ASN:HB3	2.35	0.48
2:H:163:TRP:HE1	2:H:189:ASN:CG	2.17	0.47
1:L:15:ALA:C	1:L:17:GLU:H	2.17	0.47
1:L:162:GLN:HG2	1:L:164:GLY:N	2.28	0.47
2:H:109:PHE:HD1	2:H:112:TRP:CZ2	2.32	0.47
1:L:34:ASN:HB3	1:L:36:LYS:HE3	1.43	0.47
1:L:152:VAL:HG21	1:L:181:MET:HE1	1.88	0.47
1:L:201:GLU:HB3	1:L:212:VAL:HA	1.96	0.47
2:H:49:ALA:HA	2:H:61:GLU:O	2.14	0.47
1:L:191:GLU:CA	1:L:194:ARG:HD2	2.33	0.47
1:L:153:LYS:CD	1:L:161:ARG:CD	2.89	0.47
1:L:110:LEU:HD11	1:L:112:ILE:CD1	2.43	0.47
2:H:56:ASN:C	2:H:57:LYS:O	2.53	0.47
2:H:29:PHE:C	2:H:31:ASP:H	2.18	0.47
1:L:13:VAL:O	1:L:112:ILE:HA	2.15	0.47
1:L:201:GLU:HA	1:L:212:VAL:HA	1.97	0.46
1:L:197:SER:HA	1:L:216:ASN:CB	2.41	0.46
2:H:203:SER:HA	2:H:220:VAL:O	2.15	0.46
1:L:202:ALA:O	1:L:211:ILE:N	2.32	0.46
1:L:38:PHE:HD1	1:L:38:PHE:N	2.12	0.46
1:L:5:THR:O	1:L:23:CYS:HA	2.16	0.46
1:L:110:LEU:CD1	1:L:112:ILE:CD1	2.93	0.46
1:L:104:PHE:O	4:L:303:HOH:O	2.21	0.46
1:L:176:ASP:O	1:L:177:SER:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:196:VAL:O	2:H:196:VAL:CG2	2.57	0.46
2:H:163:TRP:C	2:H:165:LYS:H	2.19	0.46
2:H:54:LYS:O	2:H:54:LYS:HD2	2.14	0.46
1:L:188:THR:O	1:L:192:TYR:N	2.33	0.46
1:L:143:ASN:O	1:L:144:ASN:HB2	2.15	0.46
2:H:134:THR:HG22	2:H:135:LEU:H	1.80	0.46
1:L:157:ASP:HA	1:L:197:SER:O	2.16	0.46
2:H:174:ASN:OD1	2:H:189:ASN:OD1	2.33	0.46
2:H:179:LEU:HD23	2:H:179:LEU:HA	1.80	0.46
2:H:6:GLU:OE2	2:H:113:GLY:CA	2.64	0.45
2:H:135:LEU:HB3	2:H:139:LEU:HD12	1.98	0.45
2:H:30:SER:O	2:H:54:LYS:HB3	2.17	0.45
1:L:151:ASN:N	1:L:151:ASN:OD1	2.47	0.45
2:H:6:GLU:OE2	2:H:114:ALA:N	2.50	0.45
2:H:29:PHE:O	2:H:31:ASP:N	2.49	0.45
1:L:19:VAL:O	1:L:80:THR:HG23	2.15	0.45
2:H:198:CYS:O	2:H:222:CYS:HB3	2.16	0.45
2:H:52:ARG:CZ	2:H:59:THR:CG2	2.94	0.45
1:L:34:ASN:HD22	1:L:36:LYS:CE	2.29	0.45
2:H:13:GLN:O	2:H:14:PRO:C	2.55	0.45
2:H:194:PRO:HB2	2:H:197:GLU:HB2	1.99	0.45
2:H:131:TYR:CB	2:H:149:LEU:HD11	2.36	0.45
1:L:201:GLU:HB3	1:L:212:VAL:CA	2.47	0.45
2:H:48:ILE:HG13	2:H:49:ALA:N	2.31	0.45
2:H:57:LYS:O	2:H:59:THR:N	2.48	0.45
1:L:187:LEU:CD1	1:L:192:TYR:CA	2.95	0.45
1:L:13:VAL:CG2	1:L:84:VAL:HG11	2.47	0.45
1:L:19:VAL:O	1:L:80:THR:HA	2.16	0.45
2:H:210:HIS:O	2:H:211:ASP:C	2.55	0.45
1:L:193:GLU:HA	1:L:218:ASN:ND2	2.33	0.44
1:L:193:GLU:HA	1:L:218:ASN:CG	2.37	0.44
1:L:123:ILE:O	2:H:135:LEU:HD21	2.18	0.44
1:L:214:SER:HB3	4:L:292:HOH:O	2.17	0.44
2:H:134:THR:CG2	2:H:221:ASN:O	2.66	0.44
1:L:128:SER:O	1:L:129:GLU:C	2.55	0.44
2:H:89:ARG:HG3	2:H:91:GLU:HG3	1.99	0.44
1:L:140:CYS:HB2	1:L:154:TRP:CZ2	2.53	0.44
1:L:87:GLU:HG3	4:L:284:HOH:O	2.16	0.44
2:H:93:THR:HA	2:H:118:VAL:O	2.18	0.44
1:L:148:LYS:O	1:L:150:ILE:HG22	2.17	0.44
2:H:56:ASN:OD1	2:H:56:ASN:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:112:ILE:H	1:L:172:GLN:NE2	2.15	0.43
1:L:142:LEU:HD13	1:L:181:MET:CG	2.48	0.43
1:L:139:VAL:HG11	2:H:133:LEU:HD21	2.00	0.43
1:L:7:SER:HA	1:L:8:PRO:C	2.38	0.43
2:H:188:SER:OG	4:H:289:HOH:O	2.21	0.43
1:L:64:VAL:HA	1:L:65:PRO:HD3	1.83	0.43
1:L:128:SER:O	1:L:132:THR:CG2	2.61	0.43
2:H:30:SER:O	2:H:31:ASP:CB	2.65	0.43
1:L:187:LEU:CD1	1:L:192:TYR:CB	2.95	0.43
1:L:96:ASN:ND2	1:L:98:HIS:HB3	2.34	0.43
2:H:205:LYS:HB2	2:H:205:LYS:HE3	1.64	0.43
2:H:78:GLN:O	2:H:79:SER:HB2	2.18	0.43
1:L:144:ASN:HA	1:L:178:THR:HB	2.01	0.42
2:H:169:ASP:HB3	2:H:194:PRO:CG	2.50	0.42
1:L:87:GLU:HG3	4:L:339:HOH:O	2.20	0.42
2:H:52:ARG:O	2:H:74:ARG:NH2	2.53	0.42
2:H:70:PHE:CD1	2:H:70:PHE:N	2.87	0.42
1:L:96:ASN:HD21	1:L:99:SER:H	1.67	0.42
1:L:45:LYS:HB3	1:L:46:PRO:CD	2.50	0.42
2:H:56:ASN:O	2:H:57:LYS:CB	2.67	0.42
1:L:172:GLN:CG	1:L:177:SER:HA	2.48	0.42
1:L:142:LEU:HD21	1:L:202:ALA:HB2	2.01	0.41
2:H:53:ASN:N	2:H:53:ASN:ND2	2.67	0.41
2:H:159:MET:HG2	2:H:187:MET:CE	2.50	0.41
2:H:52:ARG:CZ	2:H:59:THR:HG22	2.50	0.41
1:L:96:ASN:ND2	1:L:98:HIS:CB	2.84	0.41
2:H:135:LEU:HD22	2:H:139:LEU:CB	2.51	0.41
1:L:85:GLN:O	1:L:88:ASP:HB2	2.20	0.41
1:L:188:THR:OG1	1:L:191:GLU:HB3	2.14	0.41
2:H:136:PRO:O	2:H:136:PRO:HG2	2.20	0.41
2:H:56:ASN:O	2:H:57:LYS:HB2	2.21	0.41
2:H:184:ARG:HD2	2:H:184:ARG:HH11	1.56	0.41
1:L:2:ILE:HG21	1:L:2:ILE:HD13	1.54	0.41
2:H:170:ILE:HA	2:H:192:THR:O	2.20	0.41
1:L:100:TYR:HA	1:L:101:PRO:C	2.41	0.41
1:L:170:THR:HG22	1:L:180:SER:H	1.85	0.41
2:H:44:ARG:HE	2:H:44:ARG:HB3	1.72	0.41
1:L:197:SER:CB	1:L:216:ASN:HB3	2.51	0.41
1:L:131:LEU:C	1:L:133:SER:N	2.66	0.40
2:H:169:ASP:O	2:H:194:PRO:CD	2.69	0.40
2:H:200:GLU:C	2:H:202:GLU:N	2.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:187:LEU:HD11	1:L:192:TYR:HA	2.03	0.40
2:H:199:PRO:HB2	2:H:200:GLU:H	1.63	0.40
1:L:186:THR:CG2	1:L:186:THR:O	2.70	0.40
2:H:213:ASN:HB3	2:H:214:PRO:CD	2.51	0.40

All (15) 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)
1:L:132:THR:OG1	2:H:19:ARG:NH2[4_665]	1.06	1.14
1:L:15:ALA:O	2:H:1:GLU:OE2[2_665]	1.21	0.99
1:L:132:THR:OG1	2:H:19:ARG:CZ[4_665]	1.34	0.86
1:L:132:THR:CB	2:H:19:ARG:NH2[4_665]	1.41	0.79
4:H:230:HOH:O	4:H:329:HOH:O[4_664]	1.58	0.62
1:L:132:THR:CA	2:H:19:ARG:NH2[4_665]	1.89	0.31
1:L:15:ALA:O	2:H:1:GLU:CD[2_665]	1.90	0.30
1:L:15:ALA:C	2:H:1:GLU:OE2[2_665]	1.93	0.27
1:L:132:THR:O	2:H:19:ARG:NH2[4_665]	1.98	0.22
1:L:132:THR:OG1	2:H:19:ARG:NE[4_665]	1.98	0.22
1:L:132:THR:O	2:H:19:ARG:NH1[4_665]	2.00	0.20
1:L:132:THR:O	2:H:19:ARG:CZ[4_665]	2.03	0.17
1:L:18:ARG:NH1	1:L:61:GLU:OE1[2_665]	2.09	0.11
1:L:132:THR:C	2:H:19:ARG:NH1[4_665]	2.15	0.05
1:L:132:THR:C	2:H:19:ARG:NH2[4_665]	2.19	0.01

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	L	218/220 (99%)	183 (84%)	26 (12%)	9 (4%)	3 7
2	H	220/222 (99%)	192 (87%)	14 (6%)	14 (6%)	2 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	438/442 (99%)	375 (86%)	40 (9%)	23 (5%)	2 4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	132	THR
1	L	218	ASN
2	H	30	SER
2	H	31	ASP
2	H	54	LYS
2	H	168	LYS
2	H	170	ILE
2	H	199	PRO
2	H	203	SER
1	L	161	ARG
2	H	123	GLU
1	L	133	SER
1	L	158	GLY
1	L	193	GLU
2	H	57	LYS
1	L	196	ASN
1	L	217	ARG
2	H	58	TYR
2	H	137	PRO
2	H	142	ASP
2	H	48	ILE
1	L	33	GLY
2	H	55	GLY

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	L	195/195 (100%)	138 (71%)	57 (29%)	0 1
2	H	189/189 (100%)	145 (77%)	44 (23%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	384/384 (100%)	283 (74%)	101 (26%)	0 2

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	7	SER
1	L	11	LEU
1	L	19	VAL
1	L	21	MET
1	L	22	SER
1	L	28	SER
1	L	36	LYS
1	L	37	ASN
1	L	38	PHE
1	L	51	LYS
1	L	52	LEU
1	L	58	SER
1	L	60	ARG
1	L	69	THR
1	L	76	ASP
1	L	79	LEU
1	L	82	SER
1	L	89	LEU
1	L	95	GLN
1	L	96	ASN
1	L	99	SER
1	L	102	LEU
1	L	110	LEU
1	L	111	GLU
1	L	112	ILE
1	L	114	ARG
1	L	120	THR
1	L	122	SER
1	L	132	THR
1	L	133	SER
1	L	139	VAL
1	L	148	LYS
1	L	150	ILE
1	L	153	LYS
1	L	166	LEU
1	L	170	THR

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Mol	Chain	Res	Type
1	L	171	ASP
1	L	176	ASP
1	L	178	THR
1	L	181	MET
1	L	185	LEU
1	L	189	LYS
1	L	195	HIS
1	L	196	ASN
1	L	201	GLU
1	L	203	THR
1	L	205	LYS
1	L	206	THR
1	L	207	SER
1	L	211	ILE
1	L	213	LYS
1	L	214	SER
1	L	215	PHE
1	L	216	ASN
1	L	217	ARG
1	L	218	ASN
2	H	1	GLU
2	H	3	LYS
2	H	6	GLU
2	H	19	ARG
2	H	24	THR
2	H	30	SER
2	H	38	ARG
2	H	51	SER
2	H	53	ASN
2	H	54	LYS
2	H	59	THR
2	H	67	LYS
2	H	69	ARG
2	H	71	ILE
2	H	74	ARG
2	H	75	ASP
2	H	91	GLU
2	H	95	ILE
2	H	100	ARG
2	H	105	SER
2	H	106	THR
2	H	116	THR

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Mol	Chain	Res	Type
2	H	122	SER
2	H	123	GLU
2	H	127	ASN
2	H	129	THR
2	H	135	LEU
2	H	139	LEU
2	H	142	ASP
2	H	144	VAL
2	H	146	ILE
2	H	149	LEU
2	H	165	LYS
2	H	166	SER
2	H	168	LYS
2	H	179	LEU
2	H	188	SER
2	H	190	GLN
2	H	192	THR
2	H	193	LEU
2	H	197	GLU
2	H	200	GLU
2	H	209	GLN
2	H	215	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	34	ASN
1	L	37	ASN
1	L	95	GLN
1	L	96	ASN
1	L	172	GLN
1	L	195	HIS
1	L	196	ASN
1	L	216	ASN
2	H	53	ASN
2	H	101	ASN
2	H	216	GLN

5.3.3 RNA

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)

1 ligand is 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	$\#\|Z\| > 2$
3	SO4	H	223	-	4,4,4	1.12	0	6,6,6	0.22	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
3	SO4	H	223	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	223	SO4	1	0

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^{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	L	72/220 (32%)	-0.54	4 (5%) 28 26	2, 8, 27, 41	0
2	H	174/222 (78%)	-0.66	6 (3%) 49 49	2, 9, 21, 27	0
All	All	246/442 (55%)	-0.62	10 (4%) 41 41	2, 9, 23, 41	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	3	LYS	8.5
2	H	181	SER	3.2
2	H	168	LYS	3.2
1	L	220	CYS	2.9
2	H	167	GLY	2.6
1	L	186	THR	2.4
1	L	190	ASP	2.2
1	L	74	GLY	2.2
2	H	202	GLU	2.0
2	H	182	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	SO4	H	223	5/5	-	-	-	26,26,27,27	0

6.5 Other polymers

There are no such residues in this entry.