



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 08:33 am GMT

PDB ID : 3QT2  
Title : Structure of a cytokine ligand-receptor complex  
Authors : Mueller, T.D.; Patino, E.; Kotzsch, A.; Saremba, S.; Nickel, J.; Schmitz, W.;  
Sebald, W.  
Deposited on : 2011-02-22  
Resolution : 2.55 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

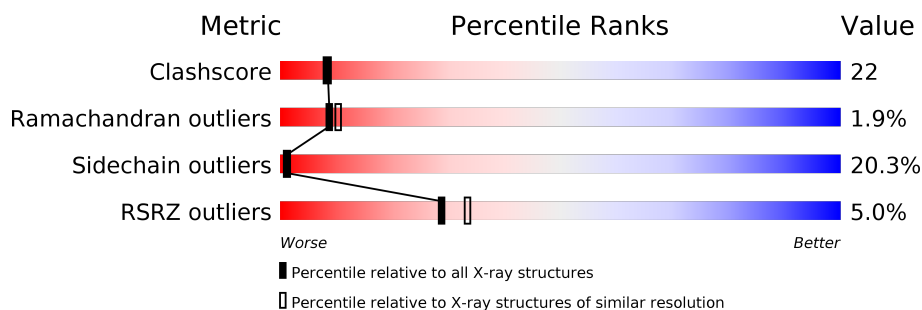
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	122126	1098 (2.56-2.52)
Ramachandran outliers	120053	1088 (2.56-2.52)
Sidechain outliers	120020	1088 (2.56-2.52)
RSRZ outliers	108989	1043 (2.56-2.52)

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	317	<div> <div>4%</div> <div>61% 27% 9% . .</div> </div>
1	B	317	<div> <div>7%</div> <div>55% 33% 9% . .</div> </div>
2	C	117	<div> <div>%</div> <div>52% 32% 10% 6%</div> </div>
2	D	117	<div> <div>6%</div> <div>44% 35% 14% 7%</div> </div>
2	E	117	<div> <div>3%</div> <div>50% 32% 11% 7%</div> </div>
2	F	117	<div> <div>4%</div> <div>53% 32% 7% . 7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BGC	A	318	-	-	-	X
3	BGC	B	317	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8581 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 Interleukin-5 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2463	1568	417	466	12			
1	B	307	Total	C	N	O	S	0	0	0
			2460	1565	416	467	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q01344
A	66	ALA	CYS	ENGINEERED MUTATION	UNP Q01344
A	72	MET	LYS	ENGINEERED MUTATION	UNP Q01344
A	138	MET	LEU	ENGINEERED MUTATION	UNP Q01344
A	167	MET	LYS	ENGINEERED MUTATION	UNP Q01344
A	234	MET	LEU	ENGINEERED MUTATION	UNP Q01344
A	313	PHE	ASN	SEE REMARK 999	UNP Q01344
A	314	SER	ASP	SEE REMARK 999	UNP Q01344
A	315	ARG	GLU	SEE REMARK 999	UNP Q01344
B	-1	MET	-	EXPRESSION TAG	UNP Q01344
B	66	ALA	CYS	ENGINEERED MUTATION	UNP Q01344
B	72	MET	LYS	ENGINEERED MUTATION	UNP Q01344
B	138	MET	LEU	ENGINEERED MUTATION	UNP Q01344
B	167	MET	LYS	ENGINEERED MUTATION	UNP Q01344
B	234	MET	LEU	ENGINEERED MUTATION	UNP Q01344
B	313	PHE	ASN	SEE REMARK 999	UNP Q01344
B	314	SER	ASP	SEE REMARK 999	UNP Q01344
B	315	ARG	GLU	SEE REMARK 999	UNP Q01344

- Molecule 2 is a protein called Interleukin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	110	Total	C	N	O	S	0	0	0
			886	563	155	165	3			

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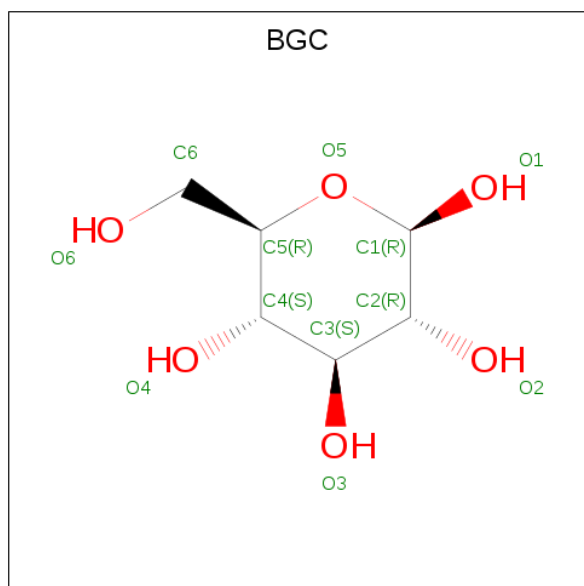
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	109	Total	C	N	O	S	0	0	0
			879	559	154	163	3			
2	E	109	Total	C	N	O	S	0	0	0
			879	559	154	163	3			
2	F	109	Total	C	N	O	S	0	0	0
			879	559	154	163	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	EXPRESSION TAG	UNP P05113
D	-1	MET	-	EXPRESSION TAG	UNP P05113
E	-1	MET	-	EXPRESSION TAG	UNP P05113
F	-1	MET	-	EXPRESSION TAG	UNP P05113

- Molecule 3 is BETA-D-GLUCOSE (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



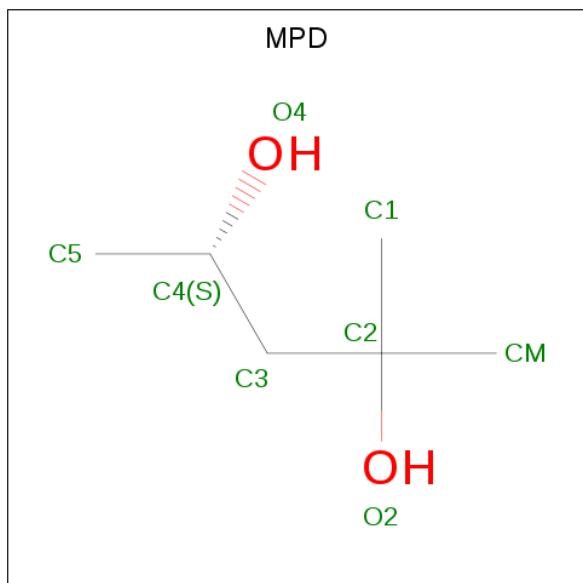
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

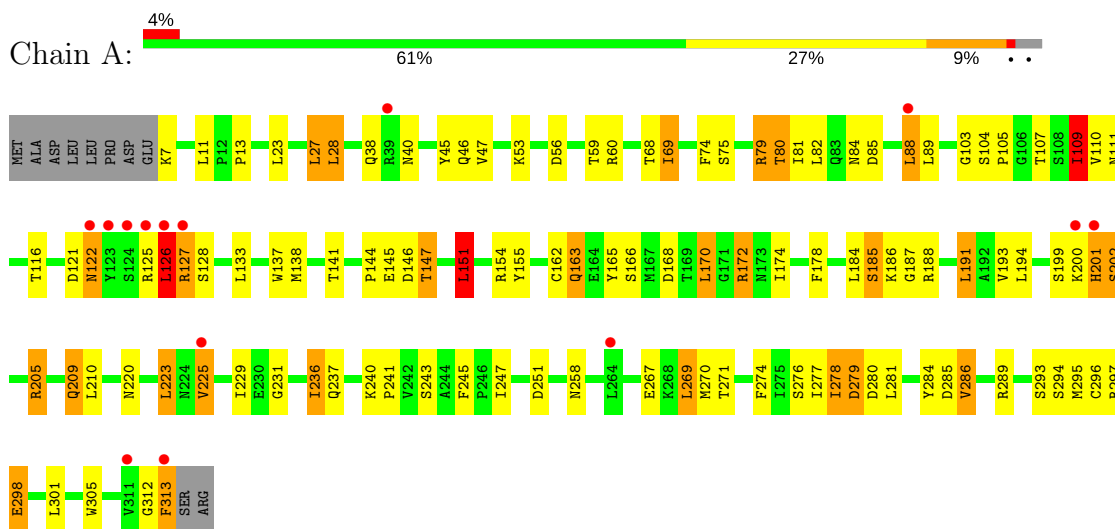
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total	O	0	0
			15	15		
5	C	8	Total	O	0	0
			8	8		
5	D	9	Total	O	0	0
			9	9		
5	B	12	Total	O	0	0
			12	12		
5	E	7	Total	O	0	0
			7	7		
5	F	4	Total	O	0	0
			4	4		

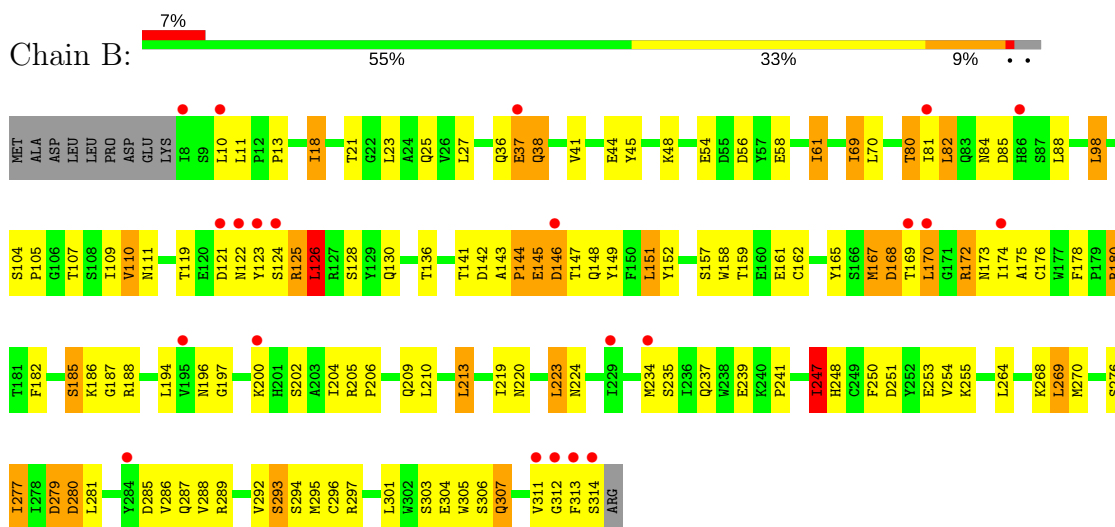
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Interleukin-5 receptor subunit alpha



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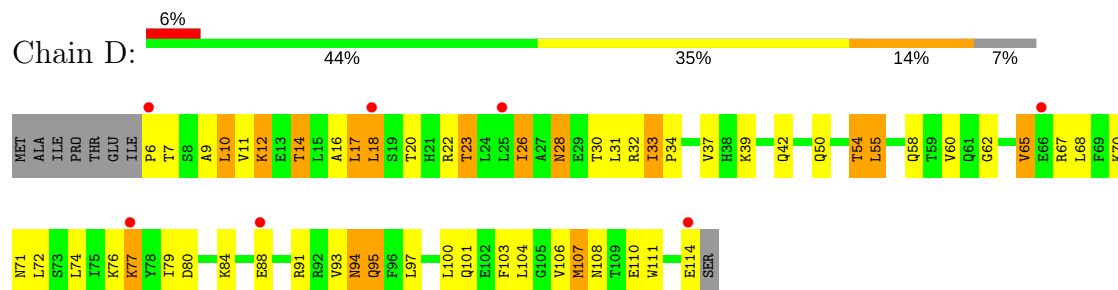


#### • Molecule 2: Interleukin-5

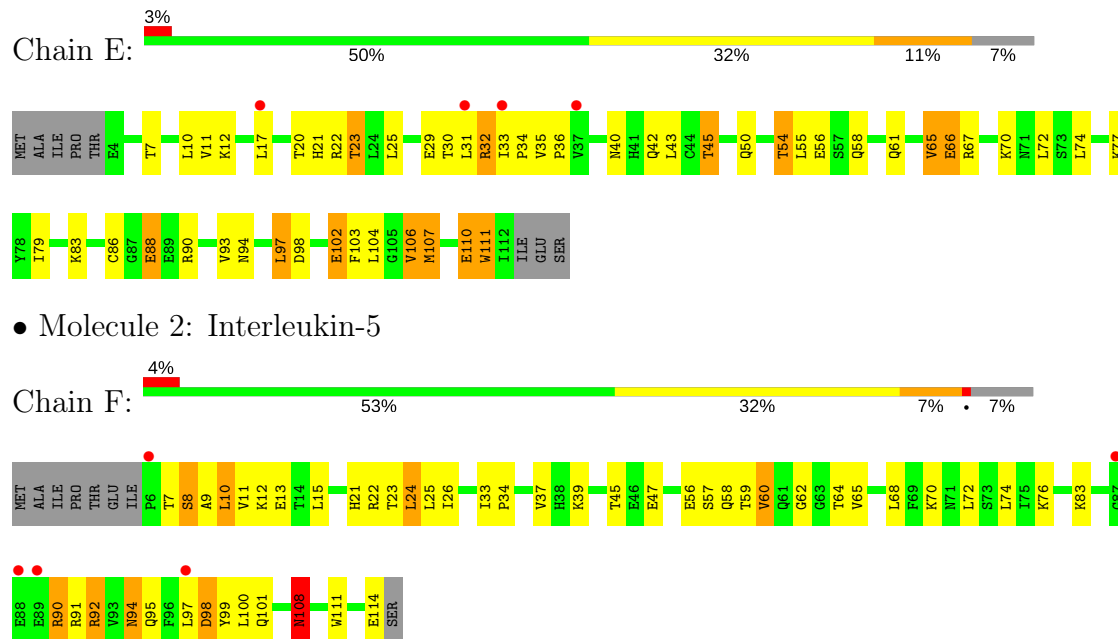




• Molecule 2: Interleukin-5



• Molecule 2: Interleukin-5





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.08Å 61.63Å 142.11Å 90.00° 99.49° 90.00°	Depositor
Resolution (Å)	42.02 – 2.55 38.49 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.02-2.55) 99.8 (38.49-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.207 , 0.264 0.210 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.48% 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: MPD, BGC

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	0.97	6/2528 (0.2%)	0.82	2/3447 (0.1%)
1	B	0.94	10/2525 (0.4%)	0.81	5/3444 (0.1%)
2	C	0.86	0/899	0.77	0/1213
2	D	0.74	0/892	0.77	0/1202
2	E	0.91	1/892 (0.1%)	0.79	0/1203
2	F	0.77	0/892	0.75	1/1202 (0.1%)
All	All	0.90	17/8628 (0.2%)	0.80	8/11711 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	GLU	CD-OE2	14.60	1.41	1.25
1	A	145	GLU	CD-OE1	14.16	1.41	1.25
1	B	170	LEU	C-N	14.04	1.58	1.33
1	B	146	ASP	CG-OD1	10.78	1.50	1.25
1	A	145	GLU	CG-CD	8.07	1.64	1.51
1	A	170	LEU	C-O	7.98	1.38	1.23
1	B	170	LEU	C-O	7.15	1.36	1.23
1	B	146	ASP	CG-OD2	7.07	1.41	1.25
1	B	145	GLU	CG-CD	6.73	1.62	1.51
1	B	172	ARG	CZ-NH1	6.72	1.41	1.33
1	B	145	GLU	CD-OE1	6.56	1.32	1.25
1	A	172	ARG	CB-CG	5.96	1.68	1.52
2	E	102	GLU	CG-CD	5.94	1.60	1.51
1	B	172	ARG	CG-CD	5.51	1.65	1.51
1	B	168	ASP	CG-OD1	5.37	1.37	1.25
1	B	145	GLU	CB-CG	5.37	1.62	1.52
1	A	172	ARG	CZ-NH2	5.29	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	LEU	CA-CB-CG	9.37	136.85	115.30
1	B	146	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	B	172	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	151	LEU	CA-CB-CG	6.03	129.16	115.30
1	B	213	LEU	CB-CG-CD1	-6.01	100.78	111.00
1	A	191	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	126	LEU	CA-CB-CG	5.23	127.33	115.30
2	F	62	GLY	N-CA-C	-5.14	100.25	113.10

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	2463	0	2389	98	0
1	B	2460	0	2381	111	0
2	C	886	0	913	55	0
2	D	879	0	907	54	0
2	E	879	0	906	49	0
2	F	879	0	907	53	0
3	A	36	0	36	0	0
3	B	36	0	36	2	0
4	A	8	0	14	0	0
5	A	15	0	0	2	0
5	B	12	0	0	1	0
5	C	8	0	0	2	0
5	D	9	0	0	2	0
5	E	7	0	0	2	0
5	F	4	0	0	1	0
All	All	8581	0	8489	376	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 22.

All (376) 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:B:123:TYR:HD2	1:B:180:ARG:NH2	0.92	1.41
1:B:295:MET:HE1	2:F:12:LYS:CD	1.58	1.31
1:A:144:PRO:O	1:A:147:THR:HG22	1.40	1.21
1:A:69:ILE:HD11	1:A:209:GLN:HA	1.23	1.18
1:B:234:MET:CE	1:B:311:VAL:HG11	1.78	1.12
2:D:26:ILE:O	2:D:26:ILE:HG12	1.39	1.12
1:B:295:MET:HE1	2:F:12:LYS:HD3	1.13	1.07
1:B:295:MET:CE	2:F:12:LYS:CD	2.32	1.06
1:A:205:ARG:HG3	1:A:205:ARG:HH11	0.93	1.05
1:A:13:PRO:HD3	1:A:80:THR:HG22	1.38	1.04
1:B:123:TYR:CD2	1:B:180:ARG:NH2	1.85	1.03
1:A:201:HIS:O	1:A:202:SER:HB3	1.55	1.03
1:A:205:ARG:HG3	1:A:205:ARG:NH1	1.72	1.00
2:C:105:GLY:O	2:C:109:THR:HG22	1.62	1.00
1:B:69:ILE:HD11	1:B:209:GLN:HA	1.44	0.99
1:A:205:ARG:CG	1:A:205:ARG:HH11	1.75	0.98
1:A:103:GLY:O	1:A:205:ARG:NH1	1.98	0.95
1:B:295:MET:CE	2:F:12:LYS:HD3	1.99	0.92
1:A:295:MET:SD	2:D:12:LYS:HG3	2.10	0.92
1:A:69:ILE:CD1	1:A:209:GLN:HA	2.00	0.92
2:C:26:ILE:HD13	2:C:26:ILE:C	1.90	0.91
1:B:234:MET:HE1	1:B:311:VAL:HG11	1.49	0.91
1:A:144:PRO:O	1:A:147:THR:CG2	2.20	0.89
1:A:46:GLN:OE1	1:A:79:ARG:NH1	2.07	0.88
2:E:35:VAL:HG11	2:F:91:ARG:HD2	1.56	0.87
2:D:22:ARG:O	2:D:26:ILE:HG22	1.73	0.87
3:B:317:BGC:H6C2	5:B:329:HOH:O	1.73	0.87
2:C:111:TRP:O	2:C:112:ILE:HB	1.74	0.86
1:A:188:ARG:NH2	1:A:296:CYS:O	2.09	0.86
1:A:278:ILE:HG13	1:A:284:TYR:CZ	2.11	0.85
1:B:295:MET:HE1	2:F:12:LYS:CG	2.07	0.85
2:E:93:VAL:HG12	2:E:97:LEU:HD22	1.59	0.85
2:F:94:ASN:O	2:F:98:ASP:OD1	1.95	0.84
1:B:152:TYR:CE2	1:B:161:GLU:HG3	2.13	0.84
2:D:94:ASN:C	2:D:94:ASN:HD22	1.81	0.84
2:C:111:TRP:HZ2	2:D:42:GLN:OE1	1.61	0.83
2:D:9:ALA:HA	5:D:123:HOH:O	1.78	0.83
1:A:295:MET:SD	2:D:12:LYS:CG	2.66	0.83
2:E:21:HIS:HD2	2:E:65:VAL:HG23	1.44	0.82
1:B:107:THR:HB	1:B:204:ILE:HG23	1.60	0.82
2:D:93:VAL:O	2:D:97:LEU:HD13	1.80	0.81
1:B:146:ASP:OD2	1:B:200:LYS:HD3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ARG:NH2	1:B:296:CYS:O	2.13	0.80
1:B:295:MET:CE	2:F:12:LYS:HD2	2.09	0.80
1:B:234:MET:CE	1:B:311:VAL:CG1	2.60	0.80
1:B:145:GLU:HA	1:B:172:ARG:HH21	1.47	0.80
2:C:100:LEU:HD22	2:C:104:LEU:HD22	1.64	0.80
2:D:26:ILE:O	2:D:26:ILE:CG1	2.27	0.80
2:D:94:ASN:HD22	2:D:95:GLN:N	1.82	0.78
2:E:32:ARG:HB3	2:F:90:ARG:HB3	1.65	0.77
1:A:295:MET:CB	2:D:12:LYS:HG2	2.15	0.76
2:E:35:VAL:HG12	2:F:91:ARG:HG3	1.68	0.75
2:F:92:ARG:HH11	2:F:92:ARG:CG	1.99	0.75
2:E:21:HIS:CD2	2:E:65:VAL:HG23	2.21	0.74
1:B:151:LEU:HD13	1:B:152:TYR:N	2.03	0.73
1:B:234:MET:HE3	1:B:311:VAL:HG11	1.70	0.73
2:D:17:LEU:HD21	2:D:67:ARG:HG2	1.70	0.73
2:C:74:LEU:HD23	2:C:74:LEU:C	2.10	0.72
2:E:98:ASP:OD1	2:F:22:ARG:NH2	2.22	0.72
2:C:100:LEU:HD22	2:C:104:LEU:CD2	2.20	0.72
2:C:10:LEU:C	2:C:10:LEU:HD23	2.10	0.71
2:D:94:ASN:ND2	2:D:95:GLN:N	2.38	0.71
1:A:201:HIS:O	1:A:202:SER:CB	2.32	0.71
2:C:41:HIS:HB3	2:D:103:PHE:HD1	1.54	0.71
1:B:234:MET:HE3	1:B:311:VAL:CG1	2.20	0.71
1:A:88:LEU:HD22	1:A:89:LEU:N	2.05	0.71
1:A:122:ASN:HA	1:A:127:ARG:HH22	1.54	0.70
2:E:35:VAL:CG1	2:F:91:ARG:HG3	2.19	0.70
1:A:267:GLU:HG3	1:A:274:PHE:CZ	2.26	0.70
1:B:36:GLN:O	1:B:38:GLN:HG3	1.92	0.70
1:A:240:LYS:HE3	1:A:245:PHE:O	1.92	0.70
1:A:137:TRP:O	1:A:174:ILE:HG12	1.93	0.69
2:C:111:TRP:CZ2	2:D:42:GLN:OE1	2.45	0.69
2:C:100:LEU:CD2	2:C:104:LEU:HD22	2.23	0.69
1:B:277:ILE:HD12	1:B:277:ILE:H	1.58	0.69
1:A:279:ASP:OD1	1:A:279:ASP:C	2.31	0.68
1:B:295:MET:HB3	2:F:12:LYS:HG3	1.76	0.67
2:F:10:LEU:HD21	2:F:74:LEU:HB2	1.76	0.67
1:A:200:LYS:HD3	1:A:200:LYS:O	1.94	0.67
2:F:37:VAL:O	2:F:37:VAL:HG12	1.92	0.67
1:A:104:SER:HB2	1:A:107:THR:HG23	1.76	0.67
1:B:197:GLY:C	1:B:204:ILE:HD12	2.14	0.67
1:A:88:LEU:CD2	1:A:89:LEU:N	2.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:ILE:O	2:C:28:ASN:N	2.26	0.66
2:E:35:VAL:HG11	2:F:91:ARG:CD	2.25	0.66
2:D:94:ASN:C	2:D:94:ASN:ND2	2.49	0.66
2:E:111:TRP:O	5:E:122:HOH:O	2.13	0.66
2:C:26:ILE:O	2:C:26:ILE:HD13	1.94	0.66
1:A:223:LEU:HD12	1:A:223:LEU:H	1.61	0.66
1:A:295:MET:SD	2:D:12:LYS:HG2	2.37	0.65
1:B:279:ASP:OD1	1:B:280:ASP:N	2.29	0.65
2:D:33:ILE:HG22	2:D:34:PRO:HD2	1.79	0.65
1:A:243:SER:HB2	5:A:321:HOH:O	1.95	0.64
2:D:37:VAL:HG23	2:D:37:VAL:O	1.98	0.64
1:A:122:ASN:OD1	1:A:122:ASN:N	2.30	0.64
2:E:35:VAL:HG13	2:E:35:VAL:O	1.97	0.64
1:A:111:ASN:HB2	1:A:138:MET:HE3	1.80	0.64
1:B:130:GLN:NE2	1:B:180:ARG:NH1	2.46	0.64
2:E:93:VAL:CG1	2:E:97:LEU:HD22	2.27	0.63
1:B:61:ILE:HD13	2:E:88:GLU:OE1	1.98	0.63
2:D:12:LYS:HD2	2:D:12:LYS:O	1.98	0.63
2:E:31:LEU:O	2:E:32:ARG:HD3	1.99	0.63
1:A:269:LEU:HD12	1:A:271:THR:OG1	1.99	0.62
2:C:105:GLY:O	2:C:109:THR:CG2	2.45	0.62
2:C:92:ARG:HG2	5:C:116:HOH:O	1.99	0.62
1:A:109:ILE:HD11	1:A:137:TRP:CD1	2.34	0.62
1:B:148:GLN:NE2	1:B:173:ASN:ND2	2.47	0.62
1:B:151:LEU:CD1	1:B:152:TYR:N	2.64	0.61
1:B:294:SER:HA	1:B:297:ARG:O	1.99	0.61
1:A:163:GLN:HB3	5:A:324:HOH:O	2.00	0.61
1:A:293:SER:OG	1:A:295:MET:HG2	2.00	0.61
1:A:121:ASP:OD1	1:A:128:SER:O	2.19	0.61
2:F:91:ARG:HD3	2:F:95:GLN:OE1	2.01	0.60
1:A:13:PRO:CD	1:A:80:THR:HG22	2.22	0.60
1:B:148:GLN:HE22	1:B:173:ASN:CG	2.04	0.60
2:E:22:ARG:HD2	2:F:97:LEU:HD23	1.84	0.60
1:B:289:ARG:HD3	1:B:305:TRP:CE2	2.37	0.60
2:F:92:ARG:HH11	2:F:92:ARG:HG3	1.66	0.60
1:A:295:MET:HB3	2:D:12:LYS:HG2	1.84	0.59
1:B:295:MET:CE	2:F:12:LYS:CG	2.76	0.59
2:E:40:ASN:ND2	2:E:111:TRP:CZ2	2.71	0.59
1:B:123:TYR:O	1:B:123:TYR:CG	2.56	0.59
1:B:105:PRO:HA	1:B:205:ARG:HH11	1.68	0.59
2:C:100:LEU:O	2:C:100:LEU:HD22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:90:ARG:HB3	2:D:32:ARG:HB3	1.83	0.58
2:E:31:LEU:C	2:E:32:ARG:HD3	2.24	0.58
1:A:144:PRO:HD2	1:A:147:THR:HG21	1.85	0.58
2:F:7:THR:O	2:F:8:SER:C	2.41	0.58
2:D:114:GLU:O	2:D:114:GLU:CG	2.51	0.58
1:B:84:ASN:OD1	1:B:85:ASP:N	2.37	0.58
1:B:279:ASP:C	1:B:279:ASP:OD1	2.42	0.58
2:C:41:HIS:HB3	2:D:103:PHE:CD1	2.37	0.58
1:B:255:LYS:HD2	1:B:264:LEU:HD11	1.86	0.58
1:A:295:MET:HB2	2:D:12:LYS:HG2	1.85	0.57
1:B:287:GLN:HG2	1:B:306:SER:O	2.04	0.57
1:B:122:ASN:OD1	1:B:125:ARG:NH2	2.38	0.57
1:A:146:ASP:OD1	1:A:199:SER:HB2	2.04	0.57
1:A:278:ILE:HG13	1:A:284:TYR:CE2	2.40	0.57
1:B:18:ILE:HG21	1:B:98:LEU:HD13	1.87	0.57
2:C:111:TRP:N	2:C:111:TRP:CD1	2.72	0.56
1:B:151:LEU:CD1	1:B:151:LEU:C	2.74	0.56
2:D:104:LEU:HD23	2:D:107:MET:CE	2.36	0.56
1:B:253:GLU:OE2	1:B:289:ARG:NH2	2.38	0.55
1:B:293:SER:OG	1:B:295:MET:HG2	2.05	0.55
1:B:48:LYS:HD3	3:B:317:BGC:O3	2.06	0.55
2:F:37:VAL:CG1	2:F:37:VAL:O	2.53	0.55
2:F:92:ARG:NH1	2:F:92:ARG:CG	2.66	0.55
1:B:130:GLN:NE2	1:B:180:ARG:HH12	2.04	0.55
2:E:35:VAL:CG1	2:F:91:ARG:HD2	2.34	0.55
1:A:88:LEU:HD23	1:A:89:LEU:H	1.71	0.55
2:D:11:VAL:HG23	2:D:12:LYS:N	2.22	0.55
2:E:36:PRO:HG2	2:F:99:TYR:CE2	2.42	0.55
1:A:312:GLY:C	1:A:313:PHE:CD1	2.80	0.55
2:D:114:GLU:O	2:D:114:GLU:HG3	2.07	0.55
1:B:10:LEU:HD11	1:B:82:LEU:HB2	1.88	0.54
1:B:295:MET:CE	2:F:12:LYS:HG3	2.38	0.54
1:B:58:GLU:OE2	2:E:90:ARG:NH1	2.40	0.54
2:F:94:ASN:C	2:F:94:ASN:HD22	2.11	0.54
2:E:50:GLN:O	2:E:54:THR:HG23	2.07	0.54
1:A:23:LEU:O	1:A:154:ARG:NH1	2.41	0.54
1:A:144:PRO:HD2	1:A:147:THR:CG2	2.37	0.54
2:C:100:LEU:O	2:C:100:LEU:CD2	2.56	0.54
2:F:24:LEU:O	2:F:24:LEU:HD12	2.08	0.53
1:B:152:TYR:CD2	1:B:161:GLU:HG3	2.42	0.53
1:B:168:ASP:O	1:B:170:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:VAL:HG11	2:F:91:ARG:CG	2.38	0.53
1:A:155:TYR:HE1	1:A:184:LEU:HD12	1.73	0.53
1:B:280:ASP:OD1	1:B:280:ASP:N	2.41	0.53
2:C:92:ARG:HD2	5:D:122:HOH:O	2.09	0.53
2:D:62:GLY:O	2:D:65:VAL:CG1	2.56	0.53
1:A:168:ASP:OD2	1:A:172:ARG:HB2	2.09	0.53
2:C:100:LEU:CD2	2:C:104:LEU:CD2	2.85	0.53
2:E:10:LEU:HD21	2:E:74:LEU:HB3	1.91	0.53
1:B:126:LEU:CD1	1:B:126:LEU:H	2.20	0.53
1:B:146:ASP:OD2	1:B:200:LYS:CD	2.55	0.53
1:B:220:ASN:O	1:B:241:PRO:HB3	2.08	0.53
2:F:68:LEU:CD2	2:F:72:LEU:HD11	2.39	0.53
1:A:151:LEU:C	1:A:151:LEU:HD12	2.29	0.52
1:A:205:ARG:NH1	1:A:205:ARG:CG	2.48	0.52
1:A:278:ILE:HG13	1:A:284:TYR:OH	2.09	0.52
1:A:88:LEU:CD2	1:A:89:LEU:H	2.22	0.52
2:C:102:GLU:O	2:C:106:VAL:HG12	2.10	0.52
2:C:93:VAL:O	2:C:94:ASN:C	2.47	0.52
2:C:92:ARG:CG	5:C:116:HOH:O	2.56	0.52
2:D:14:THR:HG21	2:D:71:ASN:HB3	1.91	0.52
2:C:106:VAL:HA	2:C:109:THR:HG23	1.91	0.52
2:C:111:TRP:HZ2	2:D:42:GLN:CD	2.13	0.51
2:D:50:GLN:O	2:D:54:THR:HG22	2.10	0.51
1:B:223:LEU:HB2	1:B:239:GLU:HB2	1.93	0.51
2:C:111:TRP:O	2:C:112:ILE:CB	2.50	0.51
1:A:312:GLY:O	1:A:313:PHE:HD1	1.94	0.51
1:A:59:THR:OG1	1:A:60:ARG:N	2.43	0.50
1:B:44:GLU:HB2	1:B:81:ILE:CG1	2.40	0.50
1:B:247:ILE:HG22	1:B:248:HIS:N	2.26	0.50
1:A:278:ILE:CG1	1:A:284:TYR:CZ	2.91	0.50
1:B:147:THR:HG22	1:B:148:GLN:N	2.26	0.50
1:A:84:ASN:C	1:A:84:ASN:OD1	2.49	0.50
2:F:10:LEU:HD21	2:F:74:LEU:CB	2.42	0.50
1:B:167:MET:HA	1:B:172:ARG:O	2.12	0.50
1:B:295:MET:HE2	2:F:12:LYS:HD2	1.91	0.50
2:C:10:LEU:HD23	2:C:11:VAL:N	2.26	0.49
2:E:93:VAL:O	2:E:94:ASN:C	2.48	0.49
1:A:109:ILE:HD11	1:A:137:TRP:NE1	2.26	0.49
2:D:10:LEU:O	2:D:14:THR:HG23	2.12	0.49
1:A:220:ASN:O	1:A:241:PRO:HB3	2.13	0.49
1:B:136:THR:HG22	1:B:175:ALA:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASP:HB2	1:B:130:GLN:HG2	1.95	0.49
2:E:36:PRO:HG2	2:F:99:TYR:CZ	2.47	0.49
1:B:224:ASN:ND2	1:B:239:GLU:OE2	2.45	0.49
2:F:21:HIS:CE1	2:F:64:THR:OG1	2.65	0.49
1:B:197:GLY:O	1:B:204:ILE:HD12	2.13	0.49
1:B:168:ASP:C	1:B:170:LEU:H	2.15	0.49
1:B:130:GLN:HG3	1:B:180:ARG:NH1	2.28	0.49
1:A:312:GLY:C	1:A:313:PHE:HD1	2.16	0.49
1:A:68:THR:HG21	1:A:74:PHE:CE1	2.48	0.49
1:B:187:GLY:C	1:B:188:ARG:HG3	2.32	0.48
2:C:6:PRO:HD3	2:C:78:TYR:CD1	2.48	0.48
1:A:289:ARG:HB2	1:A:305:TRP:CE3	2.48	0.48
1:B:61:ILE:CD1	2:E:88:GLU:OE1	2.59	0.48
1:B:21:THR:OG1	1:B:25:GLN:HG3	2.14	0.48
2:C:100:LEU:C	2:C:100:LEU:CD2	2.80	0.48
2:E:35:VAL:O	2:E:35:VAL:CG1	2.62	0.48
1:A:11:LEU:O	1:A:80:THR:HG21	2.14	0.48
2:C:29:GLU:CA	2:C:29:GLU:OE1	2.62	0.48
2:C:56:GLU:HG3	2:C:69:PHE:CD1	2.48	0.48
2:E:83:LYS:O	2:E:86:CYS:HB2	2.13	0.48
2:C:26:ILE:CD1	2:C:26:ILE:C	2.63	0.48
1:A:280:ASP:N	1:A:280:ASP:OD1	2.45	0.47
1:B:251:ASP:OD1	1:B:270:MET:HE3	2.14	0.47
1:B:88:LEU:HD23	1:B:88:LEU:C	2.34	0.47
1:B:123:TYR:CD2	1:B:123:TYR:O	2.67	0.47
1:B:18:ILE:O	1:B:18:ILE:HG22	2.12	0.47
2:D:106:VAL:C	2:D:108:ASN:H	2.16	0.47
1:A:147:THR:HB	1:A:199:SER:HB3	1.94	0.47
1:A:278:ILE:HA	1:A:278:ILE:HD12	1.64	0.47
2:C:110:GLU:C	2:C:111:TRP:HD1	2.16	0.47
1:A:274:PHE:CE2	1:A:276:SER:HB3	2.49	0.47
2:E:35:VAL:CG1	2:F:91:ARG:CG	2.87	0.47
1:A:28:LEU:HD23	1:A:28:LEU:N	2.30	0.47
1:A:125:ARG:O	1:A:126:LEU:HB2	2.15	0.47
1:A:155:TYR:CE1	1:A:184:LEU:HD12	2.49	0.47
1:A:185:SER:C	1:A:187:GLY:H	2.18	0.47
1:A:162:CYS:HB3	1:A:165:TYR:CZ	2.48	0.47
1:B:168:ASP:OD2	1:B:172:ARG:HB2	2.15	0.47
1:B:149:TYR:HA	1:B:196:ASN:O	2.13	0.47
2:C:49:PHE:CD1	2:C:76:LYS:HB2	2.49	0.47
2:E:40:ASN:ND2	2:E:43:LEU:HG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:HIS:O	2:C:22:ARG:C	2.53	0.46
1:B:130:GLN:CD	1:B:180:ARG:NH1	2.69	0.46
2:C:29:GLU:HA	2:C:29:GLU:OE1	2.15	0.46
2:D:14:THR:HG22	2:D:71:ASN:OD1	2.15	0.46
2:F:9:ALA:O	2:F:10:LEU:C	2.53	0.46
1:B:45:TYR:CE1	1:B:80:THR:HB	2.51	0.46
2:C:74:LEU:CD2	2:C:74:LEU:C	2.82	0.46
1:B:312:GLY:C	1:B:313:PHE:CD1	2.89	0.46
1:A:104:SER:HB3	1:A:105:PRO:HD2	1.98	0.46
2:E:21:HIS:CD2	2:E:65:VAL:HA	2.51	0.46
1:B:162:CYS:HB3	1:B:165:TYR:CZ	2.50	0.46
1:B:188:ARG:CZ	2:E:106:VAL:HG12	2.46	0.46
1:A:251:ASP:OD1	1:A:270:MET:HE2	2.16	0.45
2:C:8:SER:O	2:C:12:LYS:HB2	2.16	0.45
2:C:26:ILE:CD1	2:C:26:ILE:O	2.64	0.45
2:D:23:THR:HA	2:D:26:ILE:CG2	2.46	0.45
2:D:55:LEU:HA	2:D:55:LEU:HD23	1.74	0.45
1:B:125:ARG:HD3	1:B:125:ARG:HA	1.54	0.45
2:C:26:ILE:HD13	2:C:27:ALA:HA	1.98	0.45
2:D:10:LEU:HD21	2:D:74:LEU:HB2	1.99	0.45
2:C:26:ILE:HD13	2:C:27:ALA:N	2.30	0.45
2:C:33:ILE:O	2:C:34:PRO:C	2.54	0.45
2:C:97:LEU:HD12	2:C:97:LEU:HA	1.64	0.45
2:F:33:ILE:HG23	2:F:34:PRO:HD2	1.97	0.45
2:D:12:LYS:HD2	2:D:12:LYS:C	2.37	0.45
2:E:111:TRP:N	2:E:111:TRP:CD1	2.84	0.45
2:E:11:VAL:HG12	2:E:12:LYS:N	2.31	0.45
2:C:100:LEU:C	2:C:100:LEU:HD22	2.37	0.45
1:A:200:LYS:HD3	1:A:200:LYS:C	2.36	0.45
2:E:86:CYS:HB3	2:F:47:GLU:HG2	1.98	0.45
1:B:168:ASP:HB3	1:B:174:ILE:HD11	1.99	0.44
2:E:7:THR:O	2:E:10:LEU:HB3	2.17	0.44
1:B:151:LEU:C	1:B:151:LEU:HD12	2.38	0.44
2:E:45:THR:HG21	2:E:83:LYS:HE2	2.00	0.44
2:F:33:ILE:CG2	2:F:34:PRO:N	2.80	0.44
2:E:34:PRO:HG3	2:F:90:ARG:HE	1.83	0.44
2:E:104:LEU:HB2	2:F:15:LEU:HD21	1.98	0.44
1:A:13:PRO:HD3	1:A:80:THR:CG2	2.27	0.44
1:A:297:ARG:HG2	1:A:298:GLU:N	2.33	0.44
1:B:269:LEU:HD23	1:B:269:LEU:N	2.32	0.44
2:F:56:GLU:O	2:F:58:GLN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:THR:HG23	5:F:118:HOH:O	2.17	0.44
1:A:162:CYS:HA	1:A:178:PHE:CZ	2.53	0.44
1:A:313:PHE:CD1	1:A:313:PHE:N	2.82	0.44
1:B:147:THR:CG2	1:B:148:GLN:N	2.80	0.44
1:B:105:PRO:CA	1:B:205:ARG:HH11	2.30	0.44
2:C:8:SER:HB2	2:D:108:ASN:HD21	1.83	0.44
1:A:56:ASP:OD1	1:A:56:ASP:N	2.50	0.44
2:C:107:MET:HE1	2:D:79:ILE:HD11	1.99	0.44
2:F:92:ARG:HG2	2:F:92:ARG:NH1	2.32	0.44
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.84	0.44
1:B:306:SER:O	1:B:307:GLN:C	2.55	0.44
1:A:68:THR:HG21	1:A:74:PHE:CD1	2.54	0.43
2:C:10:LEU:CD2	2:C:10:LEU:C	2.83	0.43
2:E:72:LEU:HA	2:E:72:LEU:HD23	1.71	0.43
2:E:32:ARG:HD3	2:E:32:ARG:N	2.33	0.43
1:B:223:LEU:CD1	1:B:223:LEU:N	2.81	0.43
2:C:49:PHE:CE1	2:C:76:LYS:HB2	2.54	0.43
2:E:40:ASN:C	2:E:40:ASN:OD1	2.57	0.43
1:B:110:VAL:O	1:B:111:ASN:HB2	2.19	0.43
1:A:258:ASN:OD1	1:A:258:ASN:C	2.56	0.43
1:B:205:ARG:HA	1:B:206:PRO:HD2	1.92	0.43
2:C:42:GLN:HG2	2:D:111:TRP:CZ2	2.54	0.43
2:C:83:LYS:O	2:C:86:CYS:HB2	2.18	0.43
2:E:43:LEU:HA	2:E:43:LEU:HD23	1.83	0.43
2:F:92:ARG:HG2	2:F:92:ARG:HH11	1.80	0.43
1:A:121:ASP:CG	1:A:121:ASP:O	2.57	0.42
1:B:185:SER:C	1:B:187:GLY:H	2.21	0.42
1:B:219:ILE:HG22	1:B:303:SER:HB3	2.00	0.42
2:E:103:PHE:CE2	2:E:107:MET:HE1	2.53	0.42
2:C:55:LEU:HA	2:C:55:LEU:HD12	1.49	0.42
2:C:93:VAL:HG12	2:C:97:LEU:HD22	2.00	0.42
2:E:110:GLU:HB3	2:E:111:TRP:CD1	2.54	0.42
2:F:91:ARG:HB3	2:F:95:GLN:OE1	2.19	0.42
2:E:103:PHE:CZ	2:E:107:MET:HE1	2.54	0.42
1:B:269:LEU:CD2	1:B:269:LEU:N	2.81	0.42
2:D:16:ALA:O	2:D:20:THR:HG23	2.20	0.42
2:E:45:THR:HG21	2:E:83:LYS:CE	2.50	0.42
1:A:137:TRP:HZ3	1:A:151:LEU:HD23	1.83	0.42
1:B:148:GLN:HE22	1:B:173:ASN:ND2	2.15	0.42
2:D:76:LYS:HE3	2:D:80:ASP:OD1	2.19	0.42
1:B:23:LEU:HD21	1:B:152:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ARG:HD3	1:B:305:TRP:CZ2	2.54	0.42
1:A:121:ASP:O	1:A:127:ARG:NH1	2.52	0.42
1:A:278:ILE:HD11	1:A:284:TYR:CE1	2.55	0.42
1:B:279:ASP:OD1	1:B:281:LEU:N	2.49	0.42
2:D:18:LEU:HD12	2:D:68:LEU:HD11	2.02	0.42
2:E:23:THR:HG22	5:E:121:HOH:O	2.20	0.42
2:F:108:ASN:HD22	2:F:108:ASN:HA	1.68	0.41
1:B:13:PRO:HD3	1:B:80:THR:HG22	2.02	0.41
2:C:110:GLU:C	2:C:111:TRP:CD1	2.93	0.41
1:B:109:ILE:CG2	1:B:149:TYR:CE1	3.03	0.41
1:A:236:ILE:HD13	1:A:286:VAL:HG21	2.02	0.41
2:D:28:ASN:ND2	2:D:30:THR:OG1	2.53	0.41
2:D:6:PRO:HB2	2:D:7:THR:H	1.69	0.41
2:E:42:GLN:HE21	2:F:111:TRP:HE1	1.68	0.41
1:B:109:ILE:HG22	1:B:149:TYR:CE1	2.55	0.41
2:D:31:LEU:HD22	2:D:58:GLN:HG2	2.03	0.41
2:D:62:GLY:O	2:D:65:VAL:HG13	2.21	0.41
1:B:38:GLN:H	1:B:38:GLN:HG3	1.58	0.41
2:F:74:LEU:HD23	2:F:74:LEU:HA	1.84	0.41
1:A:104:SER:HB2	1:A:107:THR:CG2	2.49	0.41
1:A:109:ILE:CG1	1:A:137:TRP:CD1	3.04	0.41
1:B:176:CYS:SG	1:B:178:PHE:CE2	3.14	0.41
1:A:137:TRP:CZ3	1:A:151:LEU:HD23	2.55	0.41
1:A:289:ARG:HB2	1:A:305:TRP:CZ3	2.56	0.41
1:A:88:LEU:HD23	1:A:89:LEU:N	2.30	0.41
2:D:50:GLN:O	2:D:54:THR:CG2	2.69	0.41
2:F:33:ILE:HG22	2:F:34:PRO:N	2.34	0.41
1:A:11:LEU:O	1:A:80:THR:CG2	2.69	0.41
1:A:127:ARG:HD2	1:A:127:ARG:HA	1.42	0.41
1:A:47:VAL:O	1:A:56:ASP:HA	2.21	0.40
1:B:158:TRP:CE3	1:B:182:PHE:HB3	2.56	0.40
2:F:94:ASN:HD22	2:F:95:GLN:N	2.19	0.40
1:B:11:LEU:O	1:B:80:THR:CG2	2.70	0.40
1:B:241:PRO:HG2	1:B:250:PHE:CE2	2.57	0.40
2:D:104:LEU:HD23	2:D:107:MET:HE1	2.03	0.40
2:F:97:LEU:O	2:F:101:GLN:HG3	2.21	0.40
1:A:45:TYR:CE1	1:A:80:THR:HB	2.56	0.40
1:B:143:ALA:O	1:B:144:PRO:C	2.60	0.40
1:A:151:LEU:HD13	1:A:193:VAL:HG13	2.02	0.40
1:B:107:THR:CB	1:B:204:ILE:HG23	2.42	0.40
1:B:288:VAL:N	1:B:306:SER:OG	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:LEU:O	2:D:77:LYS:N	2.54	0.40
1:A:225:VAL:HA	1:A:237:GLN:O	2.21	0.40
1:B:234:MET:HE3	1:B:311:VAL:HG13	2.00	0.40
1:B:18:ILE:CG2	1:B:98:LEU:HD13	2.51	0.40
2:D:106:VAL:C	2:D:108:ASN:N	2.74	0.40
2:D:84:LYS:HE2	2:D:84:LYS:HB3	1.92	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	305/317 (96%)	279 (92%)	20 (7%)	6 (2%)	8	9
1	B	305/317 (96%)	281 (92%)	17 (6%)	7 (2%)	7	7
2	C	108/117 (92%)	97 (90%)	10 (9%)	1 (1%)	19	28
2	D	107/117 (92%)	96 (90%)	10 (9%)	1 (1%)	19	28
2	E	107/117 (92%)	103 (96%)	3 (3%)	1 (1%)	19	28
2	F	107/117 (92%)	99 (92%)	4 (4%)	4 (4%)	4	2
All	All	1039/1102 (94%)	955 (92%)	64 (6%)	20 (2%)	9	10

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	A	202	SER
2	C	27	ALA
1	B	169	THR
2	E	66	GLU
2	F	60	VAL

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Mol	Chain	Res	Type
1	A	186	LYS
1	B	124	SER
1	B	186	LYS
1	B	247	ILE
2	F	57	SER
2	D	10	LEU
1	B	37	GLU
1	B	144	PRO
2	F	108	ASN
1	A	85	ASP
1	B	304	GLU
2	F	8	SER
1	A	231	GLY
1	A	109	ILE

### 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	274/283 (97%)	225 (82%)	49 (18%)	2	2
1	B	274/283 (97%)	225 (82%)	49 (18%)	2	2
2	C	100/106 (94%)	79 (79%)	21 (21%)	1	1
2	D	99/106 (93%)	75 (76%)	24 (24%)	1	0
2	E	99/106 (93%)	72 (73%)	27 (27%)	0	0
2	F	99/106 (93%)	77 (78%)	22 (22%)	1	1
All	All	945/990 (96%)	753 (80%)	192 (20%)	1	1

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	27	LEU
1	A	28	LEU
1	A	38	GLN

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Mol	Chain	Res	Type
1	A	40	ASN
1	A	53	LYS
1	A	69	ILE
1	A	75	SER
1	A	79	ARG
1	A	80	THR
1	A	81	ILE
1	A	82	LEU
1	A	88	LEU
1	A	109	ILE
1	A	110	VAL
1	A	116	THR
1	A	122	ASN
1	A	126	LEU
1	A	127	ARG
1	A	133	LEU
1	A	141	THR
1	A	147	THR
1	A	151	LEU
1	A	163	GLN
1	A	166	SER
1	A	170	LEU
1	A	185	SER
1	A	191	LEU
1	A	194	LEU
1	A	201	HIS
1	A	205	ARG
1	A	209	GLN
1	A	210	LEU
1	A	223	LEU
1	A	225	VAL
1	A	229	ILE
1	A	236	ILE
1	A	247	ILE
1	A	269	LEU
1	A	277	ILE
1	A	278	ILE
1	A	279	ASP
1	A	281	LEU
1	A	285	ASP
1	A	286	VAL
1	A	294	SER

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Mol	Chain	Res	Type
1	A	298	GLU
1	A	301	LEU
1	A	313	PHE
2	C	25	LEU
2	C	26	ILE
2	C	29	GLU
2	C	30	THR
2	C	37	VAL
2	C	50	GLN
2	C	54	THR
2	C	55	LEU
2	C	57	SER
2	C	58	GLN
2	C	64	THR
2	C	68	LEU
2	C	70	LYS
2	C	74	LEU
2	C	92	ARG
2	C	97	LEU
2	C	100	LEU
2	C	104	LEU
2	C	106	VAL
2	C	109	THR
2	C	112	ILE
2	D	12	LYS
2	D	14	THR
2	D	17	LEU
2	D	18	LEU
2	D	23	THR
2	D	26	ILE
2	D	28	ASN
2	D	33	ILE
2	D	39	LYS
2	D	54	THR
2	D	55	LEU
2	D	60	VAL
2	D	65	VAL
2	D	70	LYS
2	D	72	LEU
2	D	77	LYS
2	D	88	GLU
2	D	91	ARG

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Mol	Chain	Res	Type
2	D	94	ASN
2	D	95	GLN
2	D	100	LEU
2	D	101	GLN
2	D	107	MET
2	D	110	GLU
1	B	18	ILE
1	B	27	LEU
1	B	37	GLU
1	B	38	GLN
1	B	41	VAL
1	B	54	GLU
1	B	56	ASP
1	B	61	ILE
1	B	69	ILE
1	B	70	LEU
1	B	80	THR
1	B	82	LEU
1	B	98	LEU
1	B	104	SER
1	B	110	VAL
1	B	119	THR
1	B	125	ARG
1	B	126	LEU
1	B	128	SER
1	B	141	THR
1	B	142	ASP
1	B	151	LEU
1	B	157	SER
1	B	159	THR
1	B	167	MET
1	B	180	ARG
1	B	185	SER
1	B	194	LEU
1	B	202	SER
1	B	210	LEU
1	B	213	LEU
1	B	223	LEU
1	B	235	SER
1	B	237	GLN
1	B	247	ILE
1	B	254	VAL

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Mol	Chain	Res	Type
1	B	268	LYS
1	B	269	LEU
1	B	276	SER
1	B	277	ILE
1	B	279	ASP
1	B	280	ASP
1	B	285	ASP
1	B	286	VAL
1	B	292	VAL
1	B	293	SER
1	B	301	LEU
1	B	307	GLN
1	B	314	SER
2	E	17	LEU
2	E	20	THR
2	E	23	THR
2	E	25	LEU
2	E	29	GLU
2	E	30	THR
2	E	32	ARG
2	E	33	ILE
2	E	45	THR
2	E	54	THR
2	E	55	LEU
2	E	56	GLU
2	E	58	GLN
2	E	61	GLN
2	E	65	VAL
2	E	66	GLU
2	E	67	ARG
2	E	70	LYS
2	E	77	LYS
2	E	79	ILE
2	E	88	GLU
2	E	97	LEU
2	E	102	GLU
2	E	106	VAL
2	E	107	MET
2	E	110	GLU
2	E	111	TRP
2	F	10	LEU
2	F	11	VAL

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Mol	Chain	Res	Type
2	F	13	GLU
2	F	23	THR
2	F	24	LEU
2	F	25	LEU
2	F	26	ILE
2	F	39	LYS
2	F	45	THR
2	F	59	THR
2	F	60	VAL
2	F	65	VAL
2	F	70	LYS
2	F	76	LYS
2	F	83	LYS
2	F	90	ARG
2	F	92	ARG
2	F	94	ASN
2	F	98	ASP
2	F	100	LEU
2	F	108	ASN
2	F	114	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	163	GLN
2	C	41	HIS
2	C	58	GLN
2	C	101	GLN
2	C	108	ASN
2	D	28	ASN
2	D	61	GLN
2	D	82	GLN
2	D	94	ASN
2	D	108	ASN
1	B	40	ASN
1	B	50	ASN
1	B	86	HIS
1	B	117	ASN
1	B	148	GLN
1	B	173	ASN
2	E	21	HIS

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Mol	Chain	Res	Type
2	E	42	GLN
2	E	61	GLN
2	F	21	HIS
2	F	94	ASN
2	F	101	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	$\# Z  > 2$
3	BGC	A	316	-	12,12,12	0.51	0	17,17,17	0.98	1 (5%)
3	BGC	A	317	-	12,12,12	0.61	0	17,17,17	1.27	3 (17%)
3	BGC	A	318	-	12,12,12	0.55	0	17,17,17	0.91	0
4	MPD	A	319	-	7,7,7	0.46	0	9,10,10	0.31	0
3	BGC	B	316	-	12,12,12	0.48	0	17,17,17	0.59	0
3	BGC	B	317	-	12,12,12	0.56	0	17,17,17	1.18	3 (17%)
3	BGC	B	318	-	12,12,12	0.55	0	17,17,17	0.66	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	BGC	A	316	-	-	0/2/22/22	0/1/1/1
3	BGC	A	317	-	-	0/2/22/22	0/1/1/1
3	BGC	A	318	-	-	0/2/22/22	0/1/1/1
4	MPD	A	319	-	-	0/5/5/5	0/0/0/0
3	BGC	B	316	-	-	0/2/22/22	0/1/1/1
3	BGC	B	317	-	-	0/2/22/22	0/1/1/1
3	BGC	B	318	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	317	BGC	C1-C2-C3	-2.14	106.09	110.36
3	B	317	BGC	O5-C5-C4	2.16	113.66	109.69
3	B	317	BGC	C3-C4-C5	2.20	114.18	110.24
3	A	317	BGC	C1-O5-C5	2.30	118.12	113.69
3	A	316	BGC	O5-C5-C6	2.32	112.26	106.43
3	A	317	BGC	C1-C2-C3	2.40	115.17	110.36
3	A	317	BGC	O5-C1-C2	3.08	115.85	110.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	317	BGC	2	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<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	307/317 (96%)	0.59	14 (4%)	32 39	49, 74, 120, 142	0
1	B	307/317 (96%)	0.57	22 (7%)	15 18	49, 74, 122, 153	0
2	C	110/117 (94%)	0.38	1 (0%)	84 89	51, 74, 116, 123	0
2	D	109/117 (93%)	0.52	7 (6%)	19 22	52, 86, 117, 142	0
2	E	109/117 (93%)	0.30	4 (3%)	41 48	52, 73, 103, 122	0
2	F	109/117 (93%)	0.47	5 (4%)	32 39	54, 80, 115, 135	0
All	All	1051/1102 (95%)	0.51	53 (5%)	29 33	49, 76, 118, 153	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	TYR	5.8
1	A	126	LEU	5.1
1	A	125	ARG	5.0
1	B	313	PHE	4.8
1	A	122	ASN	4.7
2	F	6	PRO	4.5
1	A	200	LYS	4.4
1	A	127	ARG	4.3
1	A	201	HIS	4.1
1	B	123	TYR	4.0
2	D	88	GLU	4.0
1	B	314	SER	3.8
2	D	6	PRO	3.6
2	F	87	GLY	3.5
1	B	86	HIS	3.5
1	B	311	VAL	3.5
1	A	39	ARG	3.5
1	B	8	ILE	3.4
2	E	37	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	97	LEU	2.9
2	C	3	THR	2.9
1	A	264	LEU	2.9
2	F	88	GLU	2.8
1	A	88	LEU	2.7
1	B	200	LYS	2.7
1	B	122	ASN	2.7
2	E	33	ILE	2.7
1	B	312	GLY	2.7
1	B	229	ILE	2.6
1	A	311	VAL	2.5
1	A	124	SER	2.4
2	D	66	GLU	2.4
2	E	31	LEU	2.4
1	A	313	PHE	2.4
1	B	37	GLU	2.4
1	B	195	VAL	2.4
1	B	10	LEU	2.4
2	F	89	GLU	2.4
1	B	169	THR	2.4
1	B	121	ASP	2.3
2	D	114	GLU	2.3
2	D	25	LEU	2.2
1	B	124	SER	2.2
1	B	81	ILE	2.2
1	B	234	MET	2.2
1	B	284	TYR	2.1
1	A	225	VAL	2.1
1	B	174	ILE	2.1
1	B	146	ASP	2.1
1	B	170	LEU	2.1
2	D	18	LEU	2.1
2	D	77	LYS	2.1
2	E	17	LEU	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 [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<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(Å <sup>2</sup> )	Q<0.9
3	BGC	A	318	12/12	0.47	0.42	128,132,134,134	0
3	BGC	B	318	12/12	0.61	0.31	129,132,133,134	0
4	MPD	A	319	8/8	0.77	0.36	104,107,110,111	0
3	BGC	B	317	12/12	0.77	0.46	139,140,142,143	0
3	BGC	A	316	12/12	0.79	0.22	118,121,122,123	0
3	BGC	A	317	12/12	0.79	0.35	117,121,122,122	0
3	BGC	B	316	12/12	0.80	0.24	115,119,120,122	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.