Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 01:27 AM EDT

PDB ID	:	3D5O
Title	:	Structural recognition and functional activation of FcrR by innate pentraxins
Authors	:	Lu, J.; Marnell, L.L.; Marjon, K.D.; Mold, C.; Du Clos, T.W.; Sun, P.D.
Deposited on	:	2008-05-16
Resolution	:	2.80 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

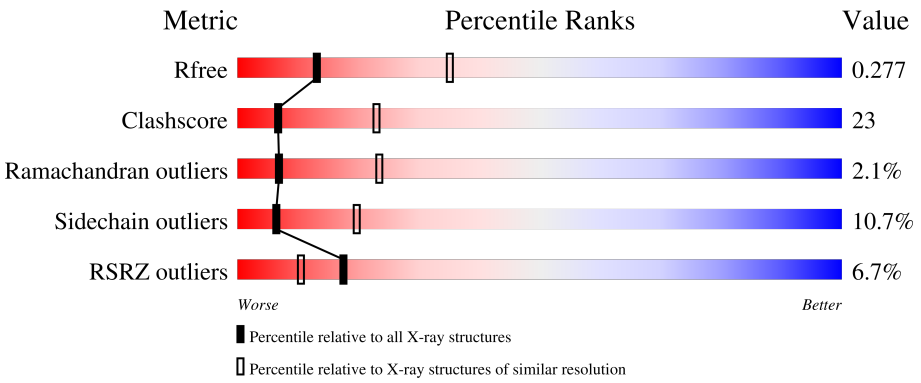
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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	204	%, 64%, 30%, 6%
1	B	204	66%, 28%, 5%
1	C	204	6%, 59%, 34%, 6%
1	D	204	7%, 53%, 40%, 7%
1	E	204	10%, 51%, 42%, 7%

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Mol	Chain	Length	Quality of chain
2	F	177	18% 49% 37% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9655 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 amyloid P-component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	204	1638	1064	268	303	3	0	0	0
1	B	204	1642	1067	269	303	3	0	0	0
1	C	204	1624	1057	263	301	3	0	0	0
1	D	204	1620	1054	262	301	3	0	0	0
1	E	204	1631	1060	265	303	3	0	0	0

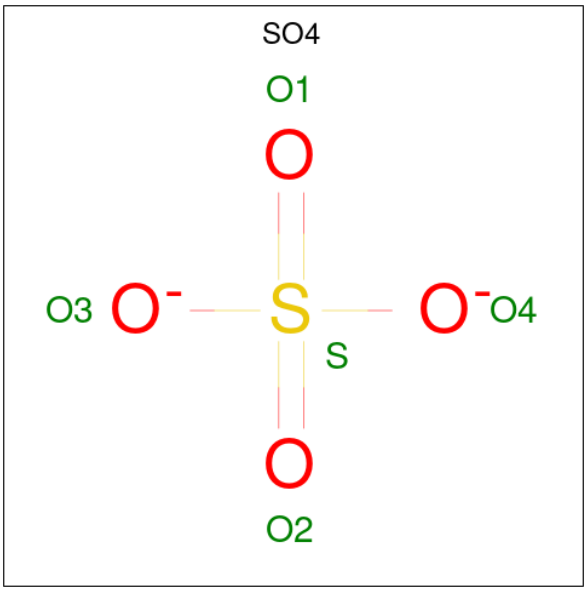
- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor II-a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	171	1313	829	226	253	5	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	131	ARG	HIS	SEE REMARK 999	UNP P12318
F	172	HIS	-	expression tag	UNP P12318
F	173	HIS	-	expression tag	UNP P12318
F	174	HIS	-	expression tag	UNP P12318
F	175	HIS	-	expression tag	UNP P12318
F	176	HIS	-	expression tag	UNP P12318
F	177	HIS	-	expression tag	UNP P12318

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



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

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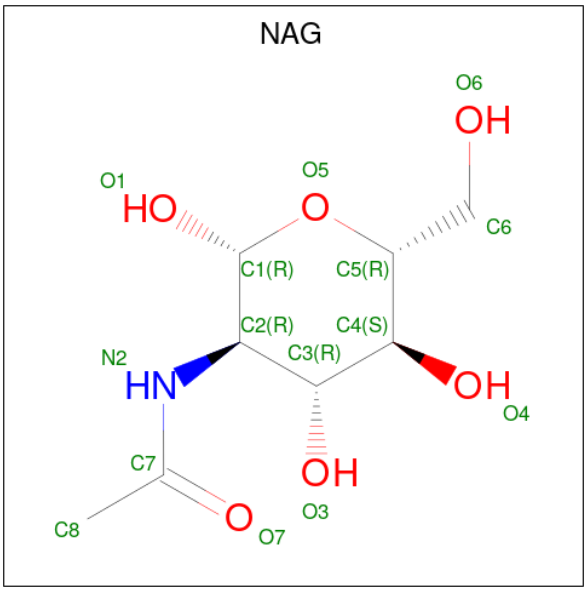
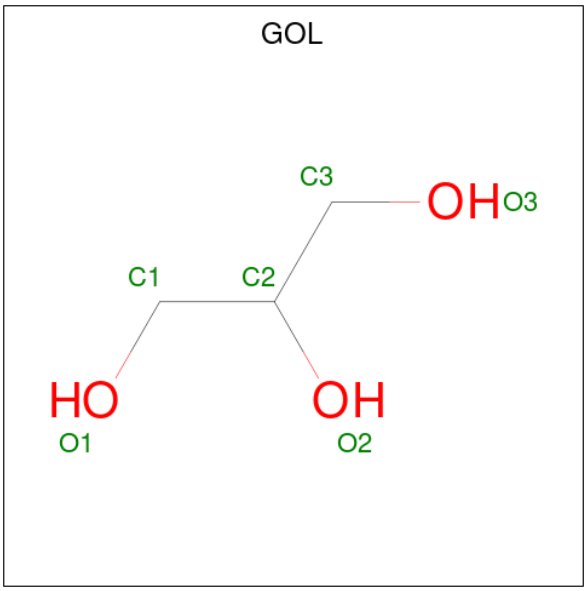
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	E	1	5	4	1		0	0
			Total	O	S			
3	F	1	5	4	1		0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
			Total	C	N	O		
4	C	1	14	8	1	5	0	0
			Total	C	N	O		
4	D	1	14	8	1	5	0	0
			Total	C	N	O		
4	E	1	14	8	1	5	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	F	1	6	3	3	0	0

- Molecule 6 is water.

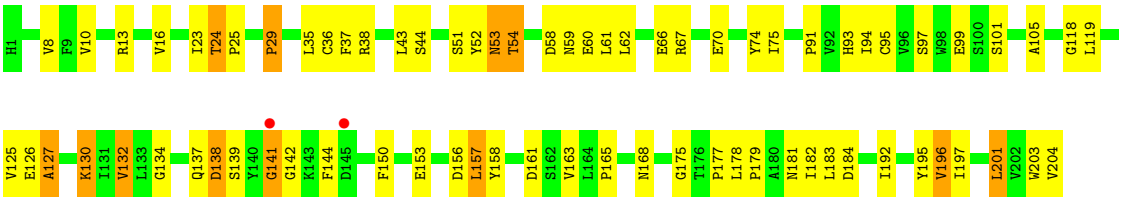
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	3	3	3	0	0
6	B	13	13	13	0	0
6	C	6	6	6	0	0
6	D	3	3	3	0	0
6	E	1	1	1	0	0
6	F	5	5	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

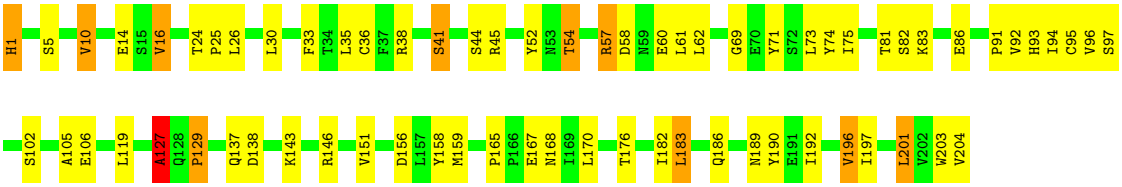
• Molecule 1: Serum amyloid P-component

Chain A:



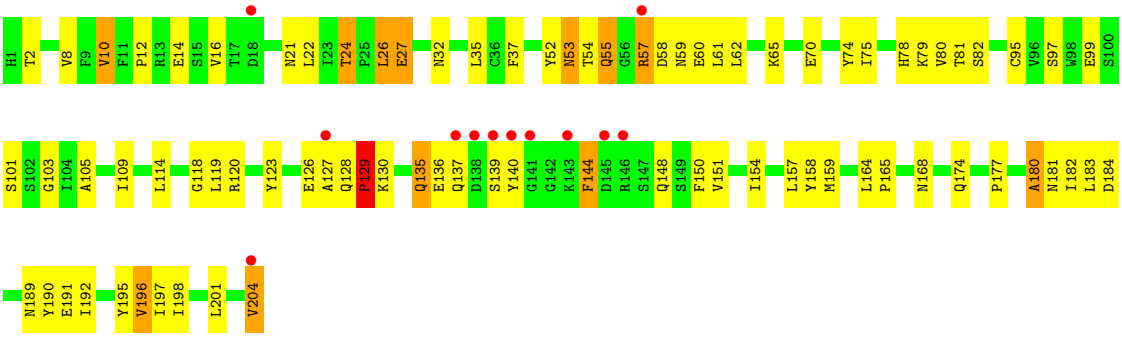
• Molecule 1: Serum amyloid P-component

Chain B:



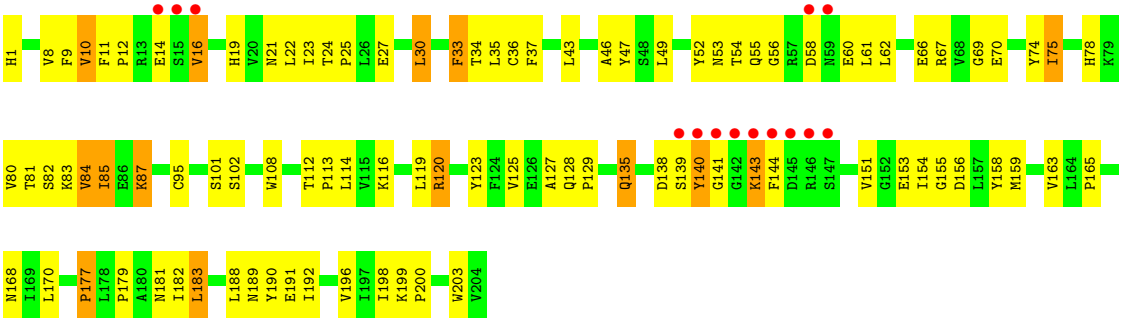
• Molecule 1: Serum amyloid P-component

Chain C:



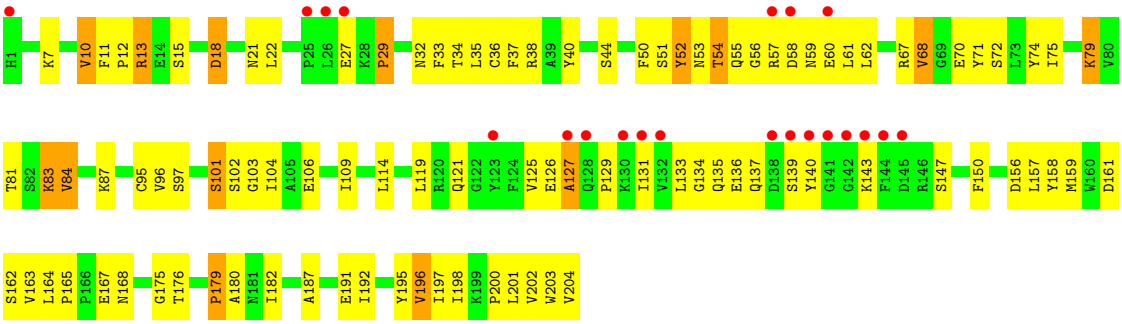
• Molecule 1: Serum amyloid P-component

Chain D:



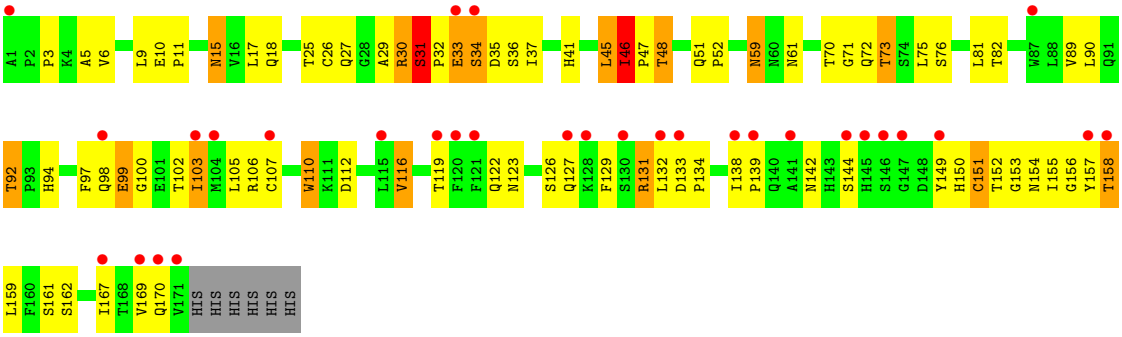
- Molecule 1: Serum amyloid P-component

Chain E:



- Molecule 2: Low affinity immunoglobulin gamma Fc region receptor II-a

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.20Å 143.48Å 161.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 47.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 97.6 (47.84-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.279 0.209 , 0.277	Depositor DCC
R_{free} test set	1471 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9655	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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 (i)

5.1 Standard geometry (i)

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

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	0.41	0/1685	0.74	1/2293 (0.0%)
1	B	0.45	0/1689	0.76	1/2297 (0.0%)
1	C	0.42	0/1671	0.74	1/2274 (0.0%)
1	D	0.40	0/1667	0.71	0/2270
1	E	0.37	0/1678	0.71	1/2284 (0.0%)
2	F	0.43	0/1351	0.79	3/1851 (0.2%)
All	All	0.41	0/9741	0.74	7/13269 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	127	ALA	N-CA-C	5.60	126.11	111.00
2	F	46	ILE	N-CA-C	-5.50	96.15	111.00
1	E	127	ALA	N-CA-C	5.23	125.11	111.00
1	A	127	ALA	N-CA-C	5.13	124.85	111.00
1	C	129	PRO	N-CA-C	5.09	125.35	112.10
2	F	33	GLU	N-CA-C	-5.05	97.36	111.00
2	F	107	CYS	CA-CB-SG	-5.03	104.94	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1638	0	1600	74	0
1	B	1642	0	1611	51	0
1	C	1624	0	1583	85	0
1	D	1620	0	1572	78	0
1	E	1631	0	1588	88	0
2	F	1313	0	1228	70	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
3	E	15	0	0	1	0
3	F	5	0	0	0	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
5	F	6	0	8	3	0
6	A	3	0	0	1	0
6	B	13	0	0	0	0
6	C	6	0	0	1	0
6	D	3	0	0	0	0
6	E	1	0	0	0	0
6	F	5	0	0	0	0
All	All	9655	0	9255	441	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 23.

All (441) 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:C:54:THR:CG2	1:C:57:ARG:HG3	1.55	1.35
1:C:54:THR:CG2	1:C:57:ARG:CG	2.15	1.23
2:F:30:ARG:NH2	2:F:72:GLN:HB2	1.64	1.13
1:C:54:THR:HG21	1:C:57:ARG:HG3	1.07	1.03
2:F:30:ARG:HH22	2:F:72:GLN:HB2	0.88	1.03
1:E:192:ILE:HG23	1:E:196:VAL:HG13	1.41	1.02
2:F:37:ILE:HD12	2:F:52:PRO:HA	1.43	1.01
1:A:130:LYS:HG2	1:A:137:GLN:NE2	1.75	1.00
1:D:52:TYR:HB3	1:D:61:LEU:HB2	1.45	0.98
1:D:192:ILE:HG23	1:D:196:VAL:HG13	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ASN:ND2	1:C:137:GLN:HG3	1.82	0.95
1:E:52:TYR:HB3	1:E:61:LEU:HB2	1.47	0.95
1:A:130:LYS:NZ	1:A:132:VAL:CG1	2.31	0.94
1:D:53:ASN:OD1	1:D:58:ASP:HA	1.68	0.93
2:F:70:THR:HB	2:F:73:THR:OG1	1.68	0.93
1:A:99:GLU:HG3	1:A:163:VAL:HG21	1.50	0.92
1:C:80:VAL:HG13	1:C:119:LEU:HD13	1.52	0.91
1:A:130:LYS:HZ3	1:A:132:VAL:CG1	1.82	0.91
1:E:38:ARG:HD2	1:E:156:ASP:OD2	1.70	0.90
1:E:34:THR:HG21	1:E:164:LEU:H	1.36	0.90
1:D:47:TYR:HE1	1:D:49:LEU:HD21	1.35	0.89
1:C:54:THR:HG21	1:C:57:ARG:CG	1.91	0.89
1:A:130:LYS:NZ	1:A:132:VAL:HG11	1.88	0.88
1:E:75:ILE:HD11	1:E:119:LEU:HG	1.53	0.88
2:F:103:ILE:HG23	2:F:138:ILE:HB	1.54	0.88
1:A:192:ILE:HG23	1:A:196:VAL:HG13	1.56	0.87
1:D:54:THR:HG22	1:D:55:GLN:H	1.39	0.86
1:C:54:THR:CG2	1:C:57:ARG:HG2	2.05	0.86
1:C:37:PHE:HB3	1:C:157:LEU:HD12	1.58	0.85
2:F:30:ARG:HH22	2:F:72:GLN:CB	1.82	0.85
2:F:45:LEU:O	2:F:47:PRO:HD3	1.77	0.84
1:B:24:THR:HG23	1:B:182:ILE:O	1.79	0.83
1:C:54:THR:HG23	1:C:57:ARG:HG2	1.59	0.83
1:E:62:LEU:HB3	1:E:74:TYR:HB2	1.59	0.83
1:A:165:PRO:HD2	1:A:168:ASN:HD22	1.42	0.83
1:D:14:GLU:HG2	1:D:151:VAL:HG21	1.60	0.82
1:E:27:GLU:O	1:E:127:ALA:HB1	1.79	0.82
1:B:127:ALA:O	1:B:129:PRO:HD3	1.80	0.81
1:C:55:GLN:HE21	1:C:128:GLN:HB2	1.44	0.81
1:A:157:LEU:HD12	1:A:158:TYR:N	1.95	0.80
1:C:54:THR:HG22	1:C:57:ARG:CG	2.10	0.80
2:F:59:ASN:C	2:F:59:ASN:HD22	1.85	0.80
1:A:130:LYS:HG2	1:A:137:GLN:HE22	1.44	0.79
1:A:137:GLN:HG2	1:A:141:GLY:HA2	1.63	0.79
1:E:134:GLY:HA2	1:E:150:PHE:HB3	1.64	0.78
1:D:21:ASN:HB2	1:D:191:GLU:HB2	1.64	0.78
1:C:24:THR:HG23	1:C:182:ILE:O	1.83	0.78
2:F:157:TYR:O	2:F:158:THR:HG23	1.82	0.78
1:A:130:LYS:HZ1	1:A:132:VAL:HG11	1.48	0.78
2:F:151:CYS:H	2:F:162:SER:HB3	1.46	0.78
1:C:54:THR:HG22	1:C:57:ARG:HG3	1.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:SER:HB2	1:B:151:VAL:O	1.84	0.77
2:F:31:SER:HB3	2:F:32:PRO:HD2	1.66	0.77
1:B:1:HIS:HB3	1:B:189:ASN:ND2	2.00	0.76
1:D:54:THR:HG22	1:D:55:GLN:N	2.01	0.76
1:D:84:VAL:HG13	1:D:114:LEU:HD21	1.68	0.75
1:E:21:ASN:HB2	1:E:191:GLU:HB2	1.68	0.75
2:F:17:LEU:HD21	2:F:89:VAL:HG23	1.68	0.75
1:A:24:THR:HG21	1:A:182:ILE:HG23	1.68	0.75
1:D:75:ILE:HG22	1:D:119:LEU:HD11	1.68	0.75
1:A:192:ILE:CG2	1:A:196:VAL:HG13	2.17	0.75
1:D:192:ILE:HG23	1:D:196:VAL:CG1	2.17	0.75
1:D:108:TRP:CZ3	1:D:113:PRO:HG3	2.22	0.74
1:B:165:PRO:HD2	1:B:168:ASN:HD22	1.52	0.74
1:C:52:TYR:HB3	1:C:61:LEU:HB2	1.71	0.73
1:A:137:GLN:HE21	1:A:141:GLY:HA2	1.54	0.73
1:D:24:THR:HG23	1:D:182:ILE:O	1.89	0.72
1:C:204:VAL:CG1	2:F:156:GLY:HA3	2.19	0.72
1:D:75:ILE:HG23	1:D:120:ARG:HG3	1.72	0.72
1:A:52:TYR:HB3	1:A:61:LEU:HB3	1.72	0.71
1:B:192:ILE:HG23	1:B:196:VAL:HG13	1.71	0.71
1:E:139:SER:HB3	1:E:143:LYS:HD2	1.73	0.71
1:C:10:VAL:O	1:C:12:PRO:HD3	1.90	0.70
1:E:60:GLU:OE2	1:E:126:GLU:HG2	1.92	0.70
2:F:34:SER:HB2	5:F:179:GOL:O3	1.92	0.70
1:C:137:GLN:NE2	1:C:144:PHE:HE1	1.89	0.69
1:E:161:ASP:HB3	1:E:182:ILE:HD11	1.74	0.69
1:C:192:ILE:HG23	1:C:196:VAL:HG13	1.73	0.69
2:F:119:THR:CG2	2:F:129:PHE:HD1	2.07	0.68
1:E:11:PHE:CE1	1:E:134:GLY:HA3	2.28	0.68
1:E:29:PRO:HD3	1:E:127:ALA:HB2	1.75	0.68
1:C:52:TYR:O	1:C:60:GLU:HB3	1.94	0.67
1:C:55:GLN:NE2	1:C:128:GLN:H	1.92	0.67
1:A:130:LYS:CG	1:A:137:GLN:NE2	2.57	0.67
2:F:15:ASN:ND2	2:F:90:LEU:O	2.27	0.67
1:A:137:GLN:HE21	1:A:141:GLY:CA	2.08	0.67
1:B:167:GLU:H	1:B:167:GLU:CD	1.98	0.67
1:D:1:HIS:HA	1:D:188:LEU:O	1.94	0.66
1:E:102:SER:HB2	1:E:104:ILE:HG12	1.75	0.66
1:A:54:THR:HG21	1:A:126:GLU:HB3	1.77	0.66
1:B:52:TYR:HB3	1:B:61:LEU:HB2	1.77	0.66
1:E:35:LEU:O	1:E:95:CYS:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:ASP:O	2:F:36:SER:HB2	1.96	0.66
1:E:159:MET:O	1:E:180:ALA:HB1	1.97	0.65
1:E:50:PHE:O	1:E:62:LEU:HD12	1.97	0.65
1:E:53:ASN:HD21	1:E:137:GLN:HB3	1.61	0.64
1:E:165:PRO:HD2	1:E:168:ASN:HD22	1.61	0.64
1:C:27:GLU:O	1:C:127:ALA:HB1	1.97	0.64
1:C:165:PRO:HD2	1:C:168:ASN:ND2	2.13	0.64
1:C:174:GLN:HA	1:C:174:GLN:NE2	2.13	0.64
1:B:75:ILE:HG13	1:B:119:LEU:HD21	1.79	0.64
1:D:54:THR:CG2	1:D:55:GLN:H	2.11	0.64
1:B:62:LEU:HB3	1:B:74:TYR:HB2	1.79	0.63
1:C:75:ILE:HG22	1:C:119:LEU:HD11	1.78	0.63
1:A:53:ASN:HD21	1:A:59:ASN:H	1.46	0.63
1:D:84:VAL:HG13	1:D:114:LEU:CD2	2.29	0.63
1:B:57:ARG:N	1:B:57:ARG:HD2	2.14	0.62
1:C:159:MET:O	1:C:182:ILE:HB	1.99	0.62
1:C:137:GLN:HE21	1:C:144:PHE:HE1	1.45	0.62
1:D:8:VAL:HG11	1:D:153:GLU:HB3	1.80	0.62
1:D:80:VAL:HG21	1:D:119:LEU:HD22	1.80	0.62
1:A:130:LYS:CG	1:A:137:GLN:HE22	2.13	0.62
1:E:192:ILE:HG23	1:E:196:VAL:CG1	2.25	0.62
1:E:35:LEU:HD11	1:E:157:LEU:HD11	1.82	0.62
2:F:152:THR:HG22	2:F:161:SER:HB3	1.80	0.62
1:A:67:ARG:NH1	1:A:70:GLU:OE2	2.32	0.62
2:F:30:ARG:HD3	2:F:70:THR:HG21	1.82	0.62
1:A:118:GLY:HA3	1:E:12:PRO:HB2	1.82	0.62
1:D:52:TYR:O	1:D:60:GLU:HB3	1.99	0.62
1:E:101:SER:O	1:E:121:GLN:HG3	2.00	0.62
1:C:74:TYR:CZ	1:C:79:LYS:HD2	2.35	0.61
1:C:135:GLN:HE21	1:C:136:GLU:H	1.46	0.61
2:F:18:GLN:HB2	2:F:110:TRP:HZ3	1.65	0.61
4:A:208:NAG:H82	4:A:208:NAG:O3	2.00	0.61
1:E:34:THR:HG21	1:E:164:LEU:N	2.11	0.61
1:C:204:VAL:HG11	2:F:156:GLY:HA3	1.81	0.61
1:E:10:VAL:O	1:E:12:PRO:HD3	2.01	0.61
1:E:192:ILE:CG2	1:E:196:VAL:HG13	2.26	0.61
1:E:54:THR:HA	1:E:140:TYR:CE1	2.36	0.60
1:D:165:PRO:HD2	1:D:168:ASN:HD22	1.67	0.60
1:E:54:THR:HA	1:E:140:TYR:HE1	1.67	0.60
1:B:176:THR:HG22	1:D:25:PRO:HB3	1.83	0.60
1:A:130:LYS:HG2	1:A:137:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:HIS:HB3	1:B:189:ASN:HD21	1.64	0.60
1:D:47:TYR:CE1	1:D:49:LEU:HD21	2.27	0.60
2:F:75:LEU:HD13	2:F:76:SER:O	2.02	0.60
1:E:67:ARG:O	1:E:68:VAL:HG23	2.01	0.60
2:F:26:CYS:HB3	2:F:37:ILE:HD13	1.82	0.59
2:F:31:SER:CB	2:F:32:PRO:HD2	2.32	0.59
1:D:8:VAL:HG13	1:D:154:ILE:O	2.02	0.59
1:E:70:GLU:HG2	1:E:83:LYS:HD2	1.85	0.59
1:A:62:LEU:HD23	1:A:74:TYR:CD1	2.38	0.58
2:F:119:THR:HG23	2:F:129:PHE:HD1	1.68	0.58
1:C:140:TYR:HB3	6:C:210:HOH:O	2.03	0.58
2:F:30:ARG:HG2	2:F:31:SER:N	2.18	0.58
1:A:35:LEU:HD11	1:A:157:LEU:HD11	1.86	0.58
2:F:153:GLY:O	2:F:159:LEU:HA	2.04	0.58
2:F:106:ARG:HA	2:F:134:PRO:O	2.04	0.58
1:C:8:VAL:HG11	1:C:201:LEU:HD13	1.86	0.57
1:A:130:LYS:HZ1	1:A:132:VAL:CG1	2.09	0.57
1:E:51:SER:OG	1:E:136:GLU:HA	2.04	0.57
2:F:97:PHE:O	2:F:169:VAL:HA	2.04	0.57
1:D:47:TYR:HE1	1:D:49:LEU:CD2	2.14	0.57
1:D:54:THR:HA	1:D:140:TYR:HE1	1.70	0.57
2:F:92:THR:HG21	2:F:167:ILE:HD11	1.86	0.57
1:A:130:LYS:NZ	1:A:132:VAL:HG12	2.19	0.57
1:C:21:ASN:HB2	1:C:191:GLU:HG3	1.85	0.57
2:F:59:ASN:C	2:F:59:ASN:ND2	2.56	0.57
1:C:60:GLU:OE1	1:C:60:GLU:HA	2.05	0.57
1:C:35:LEU:O	1:C:95:CYS:HA	2.05	0.57
1:A:8:VAL:HG13	1:A:201:LEU:HB2	1.86	0.57
1:C:150:PHE:CE2	1:C:154:ILE:HG12	2.39	0.57
1:A:197:ILE:N	1:A:197:ILE:HD12	2.19	0.57
2:F:41:HIS:HB2	2:F:46:ILE:HD11	1.86	0.56
1:A:157:LEU:HD12	1:A:157:LEU:C	2.25	0.56
1:B:24:THR:HG21	1:B:182:ILE:HG23	1.86	0.56
2:F:45:LEU:HD13	2:F:47:PRO:CA	2.36	0.56
1:D:19:HIS:HB3	1:D:135:GLN:HG3	1.87	0.56
1:C:137:GLN:NE2	1:C:144:PHE:CE1	2.71	0.56
1:D:139:SER:O	1:D:140:TYR:HB2	2.06	0.55
1:A:36:CYS:HA	1:A:94:ILE:O	2.06	0.55
1:A:29:PRO:CD	1:A:127:ALA:HB2	2.36	0.55
1:A:192:ILE:HG23	1:A:196:VAL:CG1	2.33	0.55
1:C:62:LEU:HB3	1:C:74:TYR:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ILE:CG2	1:C:196:VAL:HG13	2.37	0.55
1:E:34:THR:CG2	1:E:164:LEU:H	2.14	0.55
1:C:197:ILE:HD12	1:C:197:ILE:N	2.22	0.55
1:D:75:ILE:O	1:D:75:ILE:HD13	2.07	0.55
1:A:23:ILE:N	1:A:23:ILE:HD12	2.22	0.54
1:C:24:THR:HG21	1:C:182:ILE:HG23	1.89	0.54
1:A:53:ASN:OD1	1:A:58:ASP:HA	2.08	0.54
2:F:29:ALA:N	2:F:30:ARG:HD2	2.22	0.54
1:C:54:THR:HG22	1:C:57:ARG:CB	2.36	0.54
1:C:80:VAL:CG1	1:C:119:LEU:HD13	2.32	0.54
1:E:53:ASN:ND2	1:E:137:GLN:HB3	2.22	0.54
2:F:90:LEU:HD12	2:F:150:HIS:HA	1.90	0.54
1:D:85:ILE:HD12	1:D:85:ILE:O	2.07	0.54
1:A:58:ASP:O	1:A:59:ASN:HB2	2.07	0.54
1:E:55:GLN:N	1:E:140:TYR:CD1	2.76	0.53
2:F:15:ASN:N	2:F:15:ASN:OD1	2.41	0.53
1:B:57:ARG:HD2	1:B:57:ARG:H	1.73	0.53
1:E:51:SER:HG	1:E:136:GLU:HA	1.73	0.53
2:F:119:THR:HG23	2:F:129:PHE:CD1	2.44	0.53
1:A:130:LYS:HZ2	1:A:141:GLY:CA	2.22	0.53
2:F:29:ALA:H	2:F:30:ARG:HD2	1.73	0.53
1:D:84:VAL:CG1	1:D:114:LEU:HD21	2.39	0.53
1:E:53:ASN:HD22	1:E:58:ASP:HB2	1.73	0.53
1:B:92:VAL:HG22	1:B:93:HIS:N	2.24	0.53
1:E:60:GLU:O	1:E:75:ILE:HA	2.09	0.53
1:A:130:LYS:HZ3	1:A:132:VAL:HG12	1.69	0.52
1:B:57:ARG:HB2	1:B:60:GLU:HG2	1.91	0.52
1:C:53:ASN:HD21	1:C:137:GLN:HG3	1.67	0.52
1:E:56:GLY:O	1:E:57:ARG:HB2	2.09	0.52
1:D:33:PHE:CD1	1:D:33:PHE:C	2.82	0.52
1:D:192:ILE:CG2	1:D:196:VAL:HG13	2.30	0.52
1:D:135:GLN:HB3	1:D:144:PHE:CD1	2.45	0.52
2:F:45:LEU:O	2:F:47:PRO:CD	2.55	0.52
2:F:119:THR:HG22	2:F:129:PHE:HD1	1.74	0.52
1:D:78:HIS:CE1	1:D:120:ARG:NH2	2.78	0.52
1:C:144:PHE:HD1	1:C:144:PHE:H	1.58	0.52
1:D:8:VAL:CG1	1:D:9:PHE:N	2.73	0.51
1:E:54:THR:C	1:E:140:TYR:HD1	2.13	0.51
1:E:71:TYR:O	1:E:81:THR:HG23	2.09	0.51
1:D:75:ILE:HG23	1:D:75:ILE:O	2.09	0.51
1:E:7:LYS:HA	1:E:200:PRO:HA	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:SER:CB	2:F:32:PRO:CD	2.89	0.51
2:F:70:THR:HG22	2:F:71:GLY:N	2.26	0.51
1:A:16:VAL:O	1:A:144:PHE:HB2	2.10	0.51
1:D:70:GLU:HG2	1:D:81:THR:CG2	2.41	0.51
1:E:75:ILE:HG12	1:E:119:LEU:HD11	1.92	0.51
1:E:34:THR:HG23	1:E:163:VAL:HA	1.92	0.51
2:F:18:GLN:HB2	2:F:110:TRP:CZ3	2.46	0.51
1:A:138:ASP:HB2	1:A:142:GLY:O	2.11	0.51
1:C:81:THR:HG22	1:C:82:SER:N	2.26	0.51
1:C:55:GLN:CD	1:C:55:GLN:H	2.12	0.51
1:E:22:LEU:HB2	1:E:131:ILE:HB	1.93	0.51
1:A:195:TYR:CE1	1:A:197:ILE:HD11	2.46	0.50
2:F:10:GLU:HA	2:F:11:PRO:C	2.32	0.50
1:A:75:ILE:HG12	1:A:119:LEU:HD21	1.93	0.50
1:A:137:GLN:CG	1:A:141:GLY:HA2	2.40	0.50
1:A:161:ASP:CG	1:A:181:ASN:HD21	2.14	0.50
1:E:109:ILE:HD13	1:E:114:LEU:HD11	1.94	0.50
1:C:182:ILE:O	1:C:183:LEU:HD23	2.11	0.50
1:B:5:SER:OG	1:B:186:GLN:HG2	2.11	0.50
2:F:99:GLU:HG2	2:F:100:GLY:N	2.26	0.50
1:B:16:VAL:HG11	1:B:143:LYS:HB3	1.94	0.50
1:D:54:THR:CG2	1:D:55:GLN:N	2.70	0.49
1:E:54:THR:C	1:E:140:TYR:CD1	2.86	0.49
2:F:31:SER:HB3	2:F:32:PRO:CD	2.39	0.49
1:B:97:SER:O	1:B:105:ALA:HA	2.11	0.49
2:F:6:VAL:HB	2:F:27:GLN:HB2	1.94	0.49
2:F:45:LEU:HD13	2:F:47:PRO:HA	1.93	0.49
1:A:35:LEU:CD1	1:A:157:LEU:HD11	2.41	0.49
1:B:137:GLN:HG3	1:B:138:ASP:N	2.26	0.49
1:C:55:GLN:HE21	1:C:128:GLN:CB	2.19	0.49
2:F:149:TYR:O	2:F:150:HIS:HB3	2.13	0.49
1:D:159:MET:HB3	1:D:183:LEU:HB2	1.95	0.49
2:F:17:LEU:HD21	2:F:89:VAL:CG2	2.40	0.49
1:C:197:ILE:CG2	1:C:198:ILE:N	2.76	0.48
1:C:109:ILE:HD13	1:C:114:LEU:HD11	1.94	0.48
1:D:87:LYS:NZ	1:D:87:LYS:HB3	2.27	0.48
1:A:35:LEU:O	1:A:95:CYS:HA	2.14	0.48
1:A:158:TYR:CE2	1:A:184:ASP:OD1	2.66	0.48
1:A:196:VAL:C	1:A:197:ILE:HD12	2.33	0.48
1:C:164:LEU:HB3	1:C:168:ASN:HB2	1.95	0.48
1:A:134:GLY:HA2	1:A:150:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ASN:OD1	1:C:130:LYS:HB3	2.12	0.48
1:A:93:HIS:HD2	6:A:210:HOH:O	1.95	0.48
1:A:130:LYS:HZ2	1:A:141:GLY:HA3	1.77	0.48
1:E:75:ILE:CD1	1:E:119:LEU:HG	2.35	0.48
1:A:91:PRO:HB2	5:F:179:GOL:H12	1.95	0.48
1:C:52:TYR:O	1:C:52:TYR:HD1	1.97	0.48
1:A:24:THR:HG23	1:A:182:ILE:O	2.14	0.48
1:A:29:PRO:HD3	1:A:127:ALA:HB2	1.94	0.48
1:E:34:THR:HG23	1:E:162:SER:O	2.13	0.48
1:A:37:PHE:HA	1:A:156:ASP:O	2.12	0.47
1:D:58:ASP:C	1:D:60:GLU:H	2.16	0.47
1:E:32:ASN:O	1:E:33:PHE:HB3	2.13	0.47
1:B:38:ARG:HD2	1:B:156:ASP:OD2	2.15	0.47
1:D:8:VAL:HG12	1:D:9:PHE:N	2.29	0.47
1:E:13:ARG:HD2	1:E:13:ARG:C	2.35	0.47
1:A:53:ASN:ND2	1:A:59:ASN:H	2.10	0.47
1:B:10:VAL:HG13	1:B:197:ILE:HB	1.97	0.47
1:B:71:TYR:OH	1:B:86:GLU:OE1	2.33	0.47
1:C:180:ALA:HB3	1:C:184:ASP:HB2	1.96	0.47
1:D:138:ASP:HB2	1:D:143:LYS:HG2	1.96	0.47
1:E:135:GLN:HE21	1:E:135:GLN:HA	1.78	0.47
1:A:8:VAL:HG21	1:A:153:GLU:OE1	2.15	0.47
1:C:195:TYR:HE1	1:C:197:ILE:HD11	1.81	0.47
1:C:8:VAL:HG13	1:C:201:LEU:HB2	1.97	0.46
1:C:190:TYR:CD1	1:C:190:TYR:N	2.82	0.46
1:D:158:TYR:CZ	1:D:177:PRO:HG3	2.51	0.46
2:F:90:LEU:HD12	2:F:150:HIS:CA	2.45	0.46
1:C:32:ASN:HB3	1:C:99:GLU:HA	1.97	0.46
1:D:66:GLU:HG3	1:D:67:ARG:HG3	1.98	0.46
1:A:175:GLY:O	1:A:177:PRO:HD3	2.16	0.46
1:E:51:SER:HB3	1:E:137:GLN:HB2	1.98	0.46
1:E:75:ILE:O	1:E:75:ILE:HG13	2.15	0.46
1:C:53:ASN:ND2	1:C:137:GLN:CG	2.66	0.46
1:C:58:ASP:CG	1:C:59:ASN:H	2.19	0.46
1:C:70:GLU:OE1	1:C:81:THR:HG21	2.16	0.46
1:C:174:GLN:HA	1:C:174:GLN:HE21	1.79	0.46
1:D:23:ILE:HD12	1:D:189:ASN:C	2.36	0.46
1:E:52:TYR:CB	1:E:61:LEU:HB2	2.33	0.46
1:E:201:LEU:HD21	1:E:204:VAL:OXT	2.16	0.46
2:F:131:ARG:H	2:F:131:ARG:HG2	1.51	0.46
1:C:158:TYR:CZ	1:C:177:PRO:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:LYS:HB3	1:E:87:LYS:HE2	1.53	0.46
1:C:75:ILE:HG23	1:C:75:ILE:O	2.16	0.46
1:D:36:CYS:O	1:D:37:PHE:HB3	2.15	0.46
1:D:23:ILE:HD12	1:D:189:ASN:O	2.16	0.46
1:E:22:LEU:N	1:E:22:LEU:HD12	2.31	0.46
1:E:53:ASN:HB2	1:E:58:ASP:HA	1.98	0.46
2:F:116:VAL:O	2:F:154:ASN:HB2	2.15	0.45
1:A:38:ARG:HB3	1:A:203:TRP:HZ3	1.81	0.45
1:A:203:TRP:CD1	1:A:203:TRP:N	2.82	0.45
1:A:29:PRO:N	1:A:127:ALA:HB2	2.31	0.45
1:B:16:VAL:CG1	1:B:143:LYS:HB3	2.47	0.45
1:B:33:PHE:CD1	1:B:33:PHE:C	2.89	0.45
1:E:33:PHE:O	1:E:97:SER:HA	2.17	0.45
1:B:35:LEU:O	1:B:95:CYS:HA	2.16	0.45
1:E:34:THR:HG22	1:E:97:SER:CB	2.46	0.45
2:F:5:ALA:O	2:F:76:SER:HB2	2.16	0.45
1:E:34:THR:CG2	1:E:163:VAL:HA	2.46	0.45
2:F:119:THR:CG2	2:F:129:PHE:CD1	2.95	0.45
1:A:197:ILE:N	1:A:197:ILE:CD1	2.80	0.45
1:E:135:GLN:HE21	1:E:135:GLN:CA	2.29	0.45
1:E:52:TYR:CD1	1:E:52:TYR:C	2.90	0.45
1:C:55:GLN:NE2	1:C:128:GLN:HB2	2.22	0.45
1:B:24:THR:CG2	1:B:25:PRO:HD2	2.47	0.45
1:B:176:THR:HG22	1:B:176:THR:O	2.17	0.45
1:B:204:VAL:HG23	1:B:204:VAL:OXT	2.17	0.45
1:B:52:TYR:CB	1:B:61:LEU:HB2	2.45	0.45
1:C:78:HIS:HD2	1:C:120:ARG:NE	2.15	0.45
1:E:104:ILE:O	1:E:104:ILE:HG13	2.17	0.45
2:F:122:GLN:HG3	2:F:149:TYR:CZ	2.52	0.45
1:E:35:LEU:HD12	1:E:158:TYR:O	2.16	0.44
2:F:103:ILE:O	2:F:103:ILE:HG12	2.17	0.44
2:F:3:PRO:O	2:F:73:THR:HG22	2.17	0.44
1:A:153:GLU:CD	1:A:203:TRP:HE1	2.21	0.44
1:C:103:GLY:O	1:C:118:GLY:HA2	2.18	0.44
1:D:128:GLN:N	1:D:129:PRO:HD3	2.31	0.44
1:D:135:GLN:NE2	1:D:144:PHE:HB3	2.32	0.44
1:B:75:ILE:HG13	1:B:119:LEU:CD2	2.44	0.44
1:C:22:LEU:N	1:C:22:LEU:HD12	2.33	0.44
1:C:195:TYR:CE1	1:C:197:ILE:HD11	2.52	0.44
2:F:92:THR:HB	2:F:94:HIS:O	2.17	0.44
1:B:69:GLY:O	1:B:83:LYS:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:VAL:CG1	1:C:201:LEU:HD13	2.47	0.44
1:E:53:ASN:N	1:E:53:ASN:OD1	2.51	0.44
1:D:21:ASN:O	1:D:190:TYR:HA	2.17	0.44
2:F:89:VAL:HA	2:F:162:SER:OG	2.18	0.44
1:C:55:GLN:HE21	1:C:128:GLN:H	1.65	0.44
1:D:8:VAL:HG22	1:D:155:GLY:HA3	1.99	0.44
1:D:69:GLY:O	1:D:83:LYS:HA	2.18	0.44
1:D:199:LYS:HD3	1:D:200:PRO:HD3	1.99	0.44
1:D:87:LYS:HB3	1:D:87:LYS:HZ2	1.81	0.44
1:E:72:SER:HB3	1:E:81:THR:OG1	2.18	0.44
1:E:74:TYR:CE2	1:E:79:LYS:HB3	2.53	0.44
1:E:103:GLY:O	1:E:119:LEU:N	2.49	0.44
2:F:142:ASN:HB2	2:F:144:SER:OG	2.17	0.44
1:A:24:THR:CG2	1:A:182:ILE:HG23	2.45	0.43
1:E:167:GLU:HG3	1:E:168:ASN:N	2.31	0.43
1:B:91:PRO:HB3	1:B:203:TRP:CE3	2.53	0.43
1:B:190:TYR:CD1	1:B:190:TYR:N	2.86	0.43
1:D:140:TYR:O	1:D:140:TYR:CD2	2.71	0.43
1:E:175:GLY:O	1:E:176:THR:HG23	2.18	0.43
1:E:197:ILE:HG22	1:E:198:ILE:N	2.33	0.43
1:E:12:PRO:HG2	1:E:195:TYR:CD2	2.54	0.43
2:F:70:THR:CG2	2:F:71:GLY:N	2.82	0.43
1:D:75:ILE:HG22	1:D:119:LEU:CD1	2.46	0.43
1:A:137:GLN:NE2	1:A:141:GLY:HA2	2.27	0.43
1:B:10:VAL:HG12	1:B:197:ILE:O	2.18	0.43
1:D:27:GLU:O	1:D:127:ALA:HB1	2.18	0.43
1:D:35:LEU:O	1:D:95:CYS:HA	2.19	0.43
1:D:37:PHE:HA	1:D:156:ASP:O	2.18	0.43
1:B:14:GLU:HG3	1:B:45:ARG:HH21	1.84	0.43
1:A:51:SER:HB2	1:A:132:VAL:HG22	2.01	0.43
1:C:14:GLU:HB3	1:C:151:VAL:HG21	2.01	0.43
1:D:58:ASP:OD2	1:D:138:ASP:HA	2.19	0.43
1:D:112:THR:HA	1:D:113:PRO:HD3	1.84	0.43
1:D:199:LYS:HD3	1:D:200:PRO:CD	2.49	0.43
1:E:135:GLN:HA	1:E:135:GLN:NE2	2.34	0.42
1:B:54:THR:HB	1:B:60:GLU:HG3	2.00	0.42
1:D:30:LEU:HB2	1:D:125:VAL:HB	2.01	0.42
1:E:54:THR:OG1	1:E:126:GLU:HB2	2.18	0.42
1:B:159:MET:O	1:B:182:ILE:HB	2.19	0.42
1:A:24:THR:HG22	1:A:25:PRO:HD2	2.01	0.42
1:A:165:PRO:CD	1:A:168:ASN:HD22	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:VAL:O	1:D:144:PHE:HB2	2.20	0.42
1:D:34:THR:OG1	1:D:163:VAL:HA	2.19	0.42
1:D:81:THR:HG22	1:D:82:SER:N	2.34	0.42
1:E:61:LEU:HD23	1:E:75:ILE:HG22	2.00	0.42
1:E:84:VAL:HG22	1:E:114:LEU:CD1	2.49	0.42
2:F:105:LEU:N	2:F:105:LEU:HD12	2.34	0.42
1:B:1:HIS:HD2	1:B:1:HIS:O	2.02	0.42
1:D:75:ILE:HD13	1:D:75:ILE:C	2.40	0.42
1:D:10:VAL:O	1:D:10:VAL:CG2	2.66	0.42
1:C:54:THR:HG22	1:C:57:ARG:HB2	2.00	0.42
1:C:75:ILE:HG22	1:C:119:LEU:CD1	2.46	0.42
1:C:197:ILE:HG22	1:C:198:ILE:N	2.34	0.42
1:C:204:VAL:HG11	2:F:155:ILE:O	2.19	0.42
1:D:10:VAL:O	1:D:12:PRO:HD3	2.19	0.42
1:B:10:VAL:CG1	1:B:197:ILE:O	2.68	0.42
1:D:8:VAL:O	1:D:198:ILE:HA	2.20	0.42
1:B:36:CYS:HA	1:B:94:ILE:O	2.20	0.41
1:D:108:TRP:HA	1:D:112:THR:O	2.19	0.41
1:E:44:SER:HB3	3:E:207:SO4:O1	2.20	0.41
2:F:98:GLN:O	2:F:99:GLU:O	2.38	0.41
1:A:97:SER:O	1:A:105:ALA:HA	2.21	0.41
2:F:102:THR:HA	2:F:138:ILE:O	2.21	0.41
1:A:178:LEU:HG	1:A:179:PRO:HD2	2.02	0.41
1:C:97:SER:O	1:C:105:ALA:HA	2.20	0.41
1:E:15:SER:OG	1:E:18:ASP:HB2	2.21	0.41
1:B:92:VAL:CG2	1:B:93:HIS:N	2.84	0.41
1:D:62:LEU:HB3	1:D:74:TYR:HB2	2.02	0.41
2:F:122:GLN:OE1	2:F:127:GLN:NE2	2.53	0.41
2:F:47:PRO:HG2	2:F:48:THR:HG22	2.02	0.41
1:B:81:THR:HG22	1:B:82:SER:N	2.35	0.41
1:C:174:GLN:NE2	1:C:174:GLN:CA	2.81	0.41
1:E:54:THR:HG22	1:E:55:GLN:OE1	2.20	0.41
1:B:54:THR:HG22	1:B:57:ARG:H	1.86	0.41
1:B:158:TYR:HA	1:B:183:LEU:O	2.21	0.41
1:B:201:LEU:HD21	1:B:203:TRP:CD2	2.56	0.41
1:C:24:THR:HG22	1:C:26:LEU:H	1.86	0.41
1:E:60:GLU:HG2	1:E:125:VAL:HG13	2.03	0.41
1:B:26:LEU:HD21	1:B:30:LEU:HD13	2.02	0.41
1:B:159:MET:HG2	1:B:182:ILE:HD12	2.02	0.41
1:C:52:TYR:O	1:C:52:TYR:CD1	2.73	0.41
1:E:165:PRO:CG	1:E:168:ASN:ND2	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:CD1	1:A:179:PRO:HD2	2.51	0.40
1:A:178:LEU:HD12	1:A:179:PRO:HD2	2.02	0.40
1:E:204:VAL:OXT	1:E:204:VAL:HG12	2.21	0.40
1:C:16:VAL:O	1:C:144:PHE:HD2	2.03	0.40
1:C:120:ARG:O	1:C:123:TYR:HB3	2.21	0.40
1:A:197:ILE:HG12	1:B:102:SER:HB2	2.01	0.40
1:C:136:GLU:OE1	1:C:148:GLN:OE1	2.40	0.40
1:D:46:ALA:HB2	1:D:66:GLU:O	2.21	0.40
1:D:101:SER:OG	1:D:102:SER:N	2.54	0.40
2:F:90:LEU:HD12	2:F:150:HIS:N	2.36	0.40
1:C:57:ARG:HG2	1:C:57:ARG:H	1.38	0.40
1:D:11:PHE:CD2	1:D:11:PHE:N	2.90	0.40
1:D:165:PRO:HD2	1:D:168:ASN:ND2	2.33	0.40
1:E:10:VAL:O	1:E:12:PRO:CD	2.69	0.40
1:E:34:THR:HG22	1:E:97:SER:HB3	2.02	0.40
1:E:36:CYS:O	1:E:37:PHE:HB3	2.22	0.40
2:F:34:SER:HB2	5:F:179:GOL:C3	2.51	0.40
1:A:60:GLU:HG3	1:A:125:VAL:HG13	2.04	0.40
1:B:96:VAL:HA	1:B:106:GLU:O	2.22	0.40
1:C:158:TYR:CE1	1:C:177:PRO:HG3	2.56	0.40
1:E:52:TYR:CZ	1:E:129:PRO:HB3	2.56	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	202/204 (99%)	178 (88%)	22 (11%)	2 (1%)	15 44
1	B	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	29 61
1	C	202/204 (99%)	172 (85%)	24 (12%)	6 (3%)	4 15
1	D	202/204 (99%)	179 (89%)	17 (8%)	6 (3%)	4 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	202/204 (99%)	172 (85%)	24 (12%)	6 (3%)	4	15
2	F	169/177 (96%)	142 (84%)	23 (14%)	4 (2%)	6	20
All	All	1179/1197 (98%)	1030 (87%)	124 (10%)	25 (2%)	7	23

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	144	PHE
1	D	140	TYR
1	D	143	LYS
1	E	68	VAL
2	F	31	SER
2	F	99	GLU
1	B	127	ALA
1	C	181	ASN
1	D	56	GLY
1	E	29	PRO
1	E	59	ASN
1	C	180	ALA
1	E	18	ASP
1	E	179	PRO
1	E	187	ALA
1	C	126	GLU
1	C	139	SER
1	D	141	GLY
1	D	177	PRO
2	F	139	PRO
1	A	29	PRO
1	A	141	GLY
1	D	179	PRO
2	F	46	ILE
1	C	129	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	179/181 (99%)	161 (90%)	18 (10%)	7 22
1	B	180/181 (99%)	165 (92%)	15 (8%)	11 32
1	C	177/181 (98%)	162 (92%)	15 (8%)	10 31
1	D	176/181 (97%)	158 (90%)	18 (10%)	7 22
1	E	178/181 (98%)	161 (90%)	17 (10%)	8 24
2	F	146/163 (90%)	118 (81%)	28 (19%)	1 4
All	All	1036/1068 (97%)	925 (89%)	111 (11%)	6 20

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	13	ARG
1	A	24	THR
1	A	43	LEU
1	A	44	SER
1	A	53	ASN
1	A	54	THR
1	A	66	GLU
1	A	101	SER
1	A	130	LYS
1	A	132	VAL
1	A	138	ASP
1	A	139	SER
1	A	157	LEU
1	A	183	LEU
1	A	196	VAL
1	A	201	LEU
1	A	204	VAL
1	B	1	HIS
1	B	10	VAL
1	B	16	VAL
1	B	41	SER
1	B	44	SER
1	B	54	THR
1	B	57	ARG
1	B	58	ASP
1	B	73	LEU
1	B	129	PRO
1	B	146	ARG
1	B	170	LEU

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Mol	Chain	Res	Type
1	B	183	LEU
1	B	196	VAL
1	B	201	LEU
1	C	2	THR
1	C	10	VAL
1	C	24	THR
1	C	26	LEU
1	C	27	GLU
1	C	53	ASN
1	C	55	GLN
1	C	57	ARG
1	C	65	LYS
1	C	101	SER
1	C	129	PRO
1	C	135	GLN
1	C	189	ASN
1	C	196	VAL
1	C	204	VAL
1	D	10	VAL
1	D	16	VAL
1	D	22	LEU
1	D	30	LEU
1	D	33	PHE
1	D	43	LEU
1	D	75	ILE
1	D	84	VAL
1	D	85	ILE
1	D	87	LYS
1	D	116	LYS
1	D	120	ARG
1	D	123	TYR
1	D	135	GLN
1	D	170	LEU
1	D	181	ASN
1	D	183	LEU
1	D	203	TRP
1	E	10	VAL
1	E	13	ARG
1	E	40	TYR
1	E	52	TYR
1	E	54	THR
1	E	79	LYS

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Mol	Chain	Res	Type
1	E	83	LYS
1	E	84	VAL
1	E	96	VAL
1	E	101	SER
1	E	106	GLU
1	E	133	LEU
1	E	147	SER
1	E	179	PRO
1	E	196	VAL
1	E	202	VAL
1	E	203	TRP
2	F	9	LEU
2	F	15	ASN
2	F	25	THR
2	F	30	ARG
2	F	31	SER
2	F	33	GLU
2	F	34	SER
2	F	45	LEU
2	F	48	THR
2	F	51	GLN
2	F	59	ASN
2	F	61	ASN
2	F	73	THR
2	F	81	LEU
2	F	82	THR
2	F	92	THR
2	F	103	ILE
2	F	110	TRP
2	F	112	ASP
2	F	116	VAL
2	F	123	ASN
2	F	126	SER
2	F	131	ARG
2	F	132	LEU
2	F	133	ASP
2	F	151	CYS
2	F	158	THR
2	F	170	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	59	ASN
1	A	93	HIS
1	A	135	GLN
1	A	137	GLN
1	A	168	ASN
1	B	1	HIS
1	B	78	HIS
1	B	128	GLN
1	B	135	GLN
1	B	168	ASN
1	B	189	ASN
1	C	31	GLN
1	C	55	GLN
1	C	59	ASN
1	C	78	HIS
1	C	135	GLN
1	C	174	GLN
1	D	1	HIS
1	D	59	ASN
1	D	135	GLN
1	D	168	ASN
1	E	135	GLN
1	E	148	GLN
1	E	168	ASN
2	F	51	GLN
2	F	59	ASN
2	F	61	ASN
2	F	69	GLN
2	F	72	GLN
2	F	123	ASN
2	F	127	GLN
2	F	145	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

22 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	SO4	A	207	-	4,4,4	0.37	0	6,6,6	0.12	0
4	NAG	A	208	1	14,14,15	0.55	0	17,19,21	0.85	0
4	NAG	C	208	1	14,14,15	0.60	0	17,19,21	0.64	0
3	SO4	D	205	-	4,4,4	0.38	0	6,6,6	0.11	0
3	SO4	E	206	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	D	206	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	D	207	-	4,4,4	0.35	0	6,6,6	0.17	0
3	SO4	B	207	-	4,4,4	0.35	0	6,6,6	0.13	0
3	SO4	B	206	-	4,4,4	0.32	0	6,6,6	0.26	0
3	SO4	C	207	-	4,4,4	0.38	0	6,6,6	0.07	0
3	SO4	A	206	-	4,4,4	0.39	0	6,6,6	0.14	0
3	SO4	B	205	-	4,4,4	0.32	0	6,6,6	0.15	0
5	GOL	F	179	-	5,5,5	0.28	0	5,5,5	0.32	0
3	SO4	A	205	-	4,4,4	0.36	0	6,6,6	0.14	0
4	NAG	E	208	1	14,14,15	0.78	1 (7%)	17,19,21	0.93	1 (5%)
3	SO4	C	206	-	4,4,4	0.39	0	6,6,6	0.18	0
3	SO4	E	207	-	4,4,4	0.35	0	6,6,6	0.07	0
4	NAG	B	208	1	14,14,15	0.63	0	17,19,21	0.67	0
3	SO4	C	205	-	4,4,4	0.39	0	6,6,6	0.14	0
4	NAG	D	208	1	14,14,15	0.72	0	17,19,21	0.60	0
3	SO4	F	178	-	4,4,4	0.35	0	6,6,6	0.18	0
3	SO4	E	205	-	4,4,4	0.41	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	208	1	-	3/6/23/26	0/1/1/1
4	NAG	C	208	1	-	3/6/23/26	0/1/1/1
4	NAG	B	208	1	-	4/6/23/26	0/1/1/1
4	NAG	D	208	1	-	3/6/23/26	0/1/1/1
5	GOL	F	179	-	-	0/4/4/4	-
4	NAG	E	208	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	208	NAG	C1-C2	2.02	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	208	NAG	C2-N2-C7	-2.12	120.06	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	208	NAG	C3-C2-N2-C7
4	A	208	NAG	C8-C7-N2-C2
4	A	208	NAG	O7-C7-N2-C2
4	B	208	NAG	C3-C2-N2-C7
4	C	208	NAG	C8-C7-N2-C2
4	C	208	NAG	O7-C7-N2-C2
4	E	208	NAG	C8-C7-N2-C2
4	E	208	NAG	O7-C7-N2-C2
4	B	208	NAG	C8-C7-N2-C2
4	B	208	NAG	O7-C7-N2-C2
4	C	208	NAG	C3-C2-N2-C7
4	B	208	NAG	O5-C5-C6-O6
4	D	208	NAG	C1-C2-N2-C7
4	D	208	NAG	C3-C2-N2-C7
4	D	208	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	208	NAG	1	0
5	F	179	GOL	3	0
3	E	207	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	204/204 (100%)	0.02	2 (0%) 82 77	19, 36, 69, 111	0
1	B	204/204 (100%)	-0.26	0 100 100	20, 34, 57, 77	0
1	C	204/204 (100%)	0.30	12 (5%) 22 14	24, 47, 93, 119	0
1	D	204/204 (100%)	0.25	14 (6%) 16 10	31, 51, 95, 120	0
1	E	204/204 (100%)	0.50	21 (10%) 6 3	27, 58, 93, 117	0
2	F	171/177 (96%)	0.83	31 (18%) 1 1	20, 68, 92, 109	0
All	All	1191/1197 (99%)	0.26	80 (6%) 17 10	19, 48, 91, 120	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	141	GLY	12.5
1	C	140	TYR	11.7
1	C	139	SER	9.5
1	D	145	ASP	8.0
1	D	143	LYS	7.6
1	D	142	GLY	7.5
1	D	144	PHE	6.4
1	E	141	GLY	6.4
2	F	157	TYR	6.0
1	E	140	TYR	5.6
2	F	132	LEU	5.2
1	D	141	GLY	5.1
1	A	141	GLY	5.0
2	F	169	VAL	5.0
2	F	139	PRO	4.7
1	C	127	ALA	4.5
1	E	131	ILE	4.2
1	E	128	GLN	4.2
1	E	142	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	58	ASP	4.0
1	E	27	GLU	3.7
2	F	145	HIS	3.6
1	E	26	LEU	3.5
2	F	120	PHE	3.5
2	F	104	MET	3.4
2	F	33	GLU	3.4
1	C	204	VAL	3.4
1	E	25	PRO	3.4
1	E	139	SER	3.4
1	E	144	PHE	3.4
1	C	146	ARG	3.3
1	D	58	ASP	3.3
2	F	121	PHE	3.3
2	F	1	ALA	3.3
2	F	171	VAL	3.3
1	C	145	ASP	3.3
1	D	139	SER	3.3
2	F	34	SER	3.2
2	F	130	SER	3.2
1	E	138	ASP	3.1
2	F	127	GLN	3.1
1	E	143	LYS	3.0
2	F	170	GLN	3.0
2	F	98	GLN	2.9
1	D	146	ARG	2.8
1	D	147	SER	2.8
1	E	132	VAL	2.8
1	D	140	TYR	2.8
2	F	144	SER	2.7
1	E	1	HIS	2.7
2	F	119	THR	2.6
2	F	158	THR	2.6
1	C	18	ASP	2.6
2	F	87	TRP	2.6
2	F	167	ILE	2.5
2	F	103	ILE	2.5
1	E	130	LYS	2.5
1	D	59	ASN	2.4
1	D	16	VAL	2.4
1	C	138	ASP	2.3
2	F	128	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	115	LEU	2.3
1	E	60	GLU	2.3
2	F	107	CYS	2.3
2	F	133	ASP	2.3
1	A	145	ASP	2.2
2	F	138	ILE	2.2
1	C	137	GLN	2.2
1	C	143	LYS	2.2
2	F	146	SER	2.2
1	E	145	ASP	2.1
2	F	147	GLY	2.1
1	C	57	ARG	2.1
1	D	14	GLU	2.1
1	E	127	ALA	2.1
1	D	15	SER	2.1
2	F	149	TYR	2.1
2	F	141	ALA	2.0
1	E	123	TYR	2.0
1	E	57	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	NAG	B	208	14/15	0.74	0.28	48,64,79,92	0
4	NAG	D	208	14/15	0.75	0.27	56,74,84,91	0
4	NAG	C	208	14/15	0.77	0.26	64,76,85,86	0
5	GOL	F	179	6/6	0.77	0.28	48,63,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	205	5/5	0.83	0.26	81,83,87,94	0
3	SO4	D	205	5/5	0.83	0.18	82,82,94,96	0
4	NAG	E	208	14/15	0.85	0.31	67,78,87,91	0
4	NAG	A	208	14/15	0.86	0.17	53,67,80,82	0
3	SO4	C	206	5/5	0.86	0.16	77,82,86,93	0
3	SO4	E	206	5/5	0.86	0.20	85,85,89,91	0
3	SO4	E	205	5/5	0.88	0.18	73,75,92,95	0
3	SO4	D	206	5/5	0.91	0.17	67,76,84,85	0
3	SO4	A	207	5/5	0.91	0.19	61,63,71,74	0
3	SO4	C	205	5/5	0.91	0.16	62,71,75,83	0
3	SO4	A	205	5/5	0.93	0.12	69,69,79,89	0
3	SO4	F	178	5/5	0.93	0.15	73,76,80,87	0
3	SO4	D	207	5/5	0.94	0.12	76,77,86,88	0
3	SO4	A	206	5/5	0.95	0.12	66,67,74,74	0
3	SO4	E	207	5/5	0.95	0.18	75,75,79,80	0
3	SO4	C	207	5/5	0.95	0.21	72,80,85,85	0
3	SO4	B	206	5/5	0.97	0.19	48,57,63,68	0
3	SO4	B	207	5/5	0.97	0.11	67,68,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.