Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:00 AM GMT

PDB ID	:	3KGL
Title	:	Crystal structure of procruciferin, 11S globulin from Brassica napus
Authors	:	Tandang-Silvas, M.R.; Mikami, B.; Maruyama, N.; Utsumi, S.
Deposited on	:	2009-10-29
Resolution	:	2.98 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:

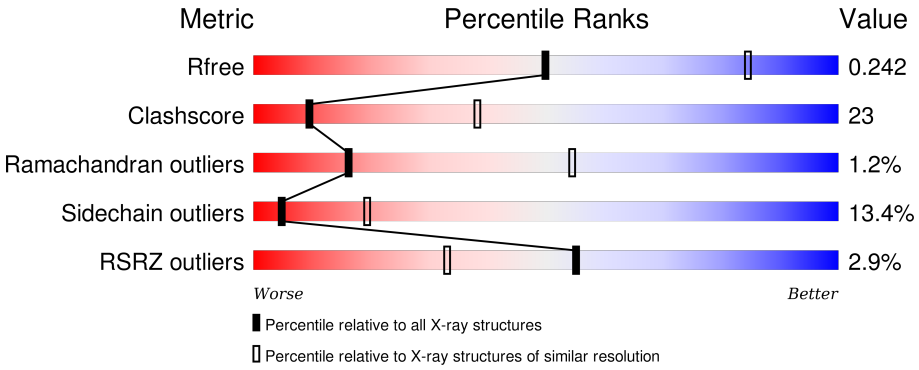
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.98 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}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	A	466	4% 47% 33% 6% 15%
1	B	466	2% 45% 32% 6% 17%
1	C	466	% 47% 30% 6% 17%
1	D	466	2% 48% 32% • 16%
1	E	466	2% 48% 29% 7% 17%

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Mol	Chain	Length	Quality of chain
1	F	466	4% 45% 34% 6% 15%

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
2	GOL	D	467	-	-	X	-
2	GOL	E	467	-	-	X	-
3	SO4	A	474	-	-	-	X
3	SO4	D	473	-	-	-	X

2 Entry composition

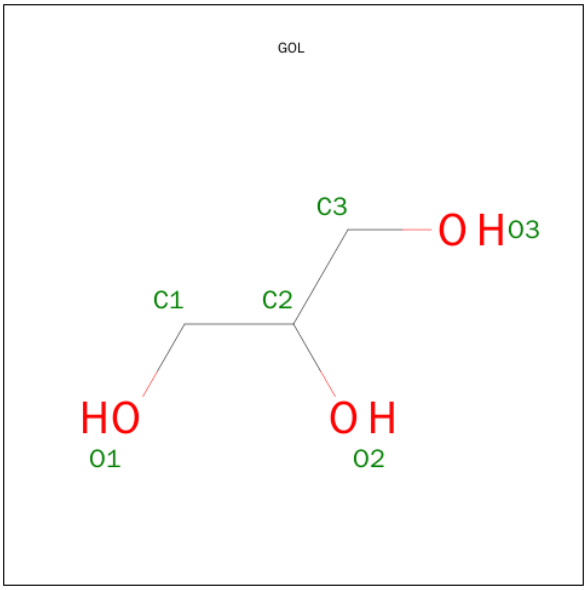
There are 4 unique types of molecules in this entry. The entry contains 18711 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cruciferin.

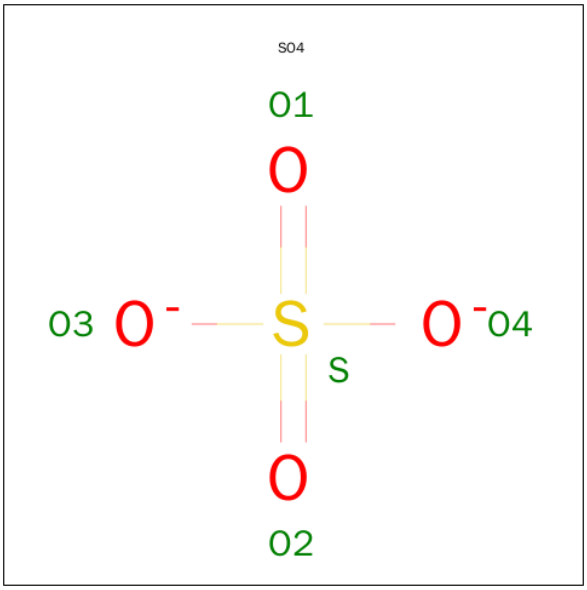
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3134	1969	569	588	8			
1	B	387	Total	C	N	O	S	0	0	0
			3042	1909	554	571	8			
1	C	387	Total	C	N	O	S	0	0	0
			3046	1909	556	573	8			
1	D	390	Total	C	N	O	S	0	0	0
			3067	1923	561	575	8			
1	E	389	Total	C	N	O	S	0	0	0
			3061	1920	558	575	8			
1	F	396	Total	C	N	O	S	0	1	0
			3119	1958	568	585	8			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- 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	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

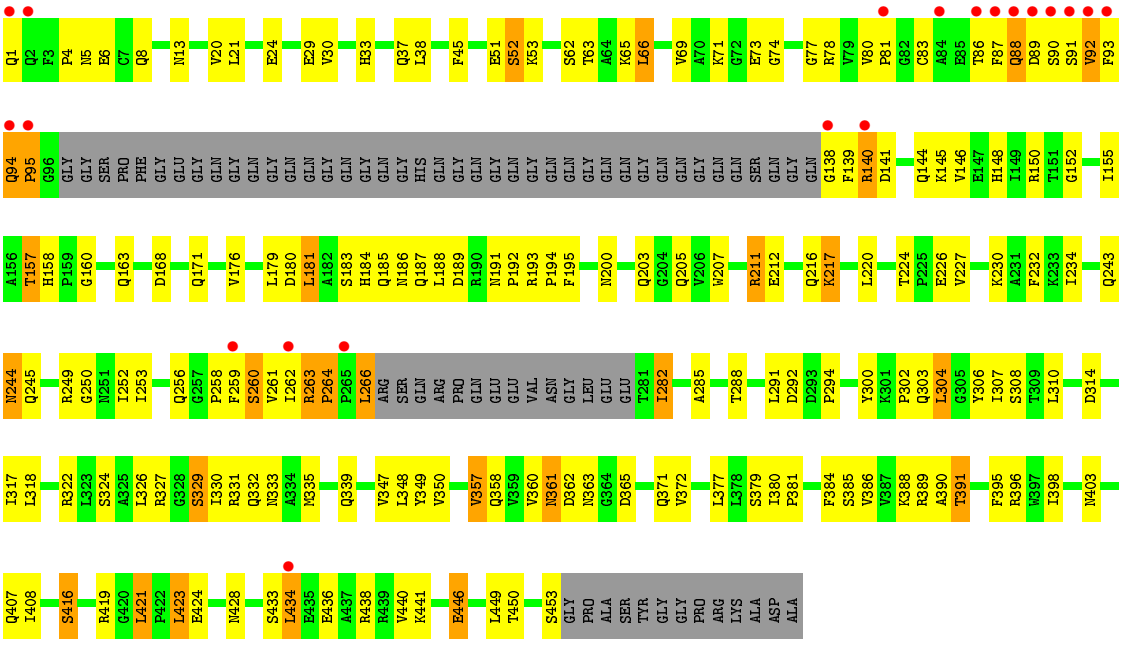
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	37	Total O 37 37	0	0
4	C	25	Total O 25 25	0	0
4	D	44	Total O 44 44	0	0
4	E	27	Total O 27 27	0	0
4	F	24	Total O 24 24	0	0

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.

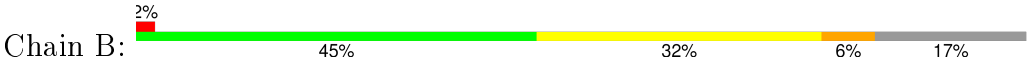
- Molecule 1: Cruciferin

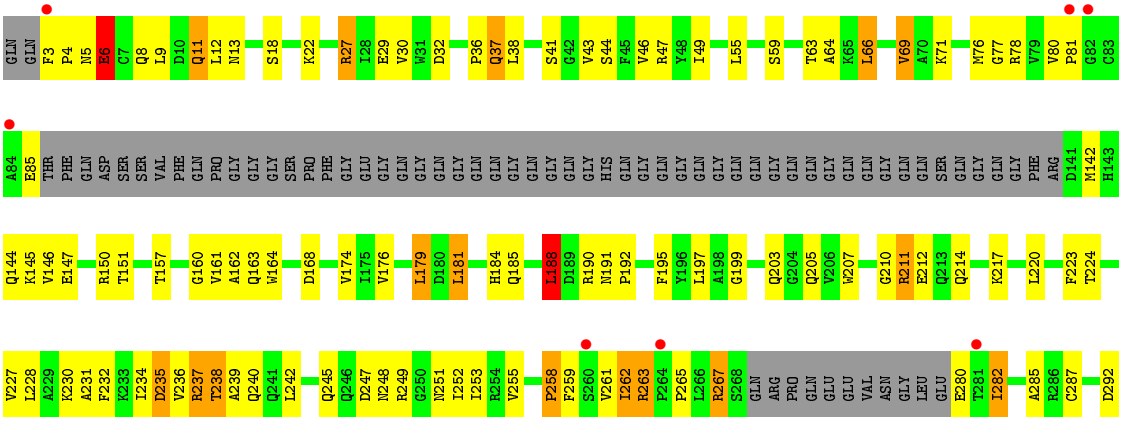
Chain A:

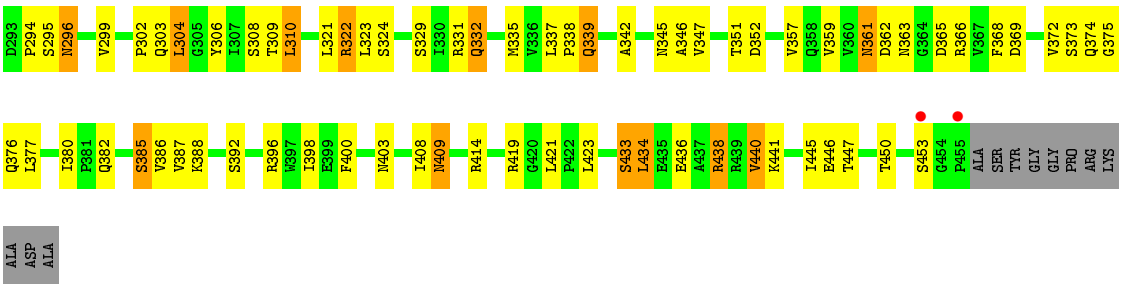


- Molecule 1: Cruciferin

Chain B:

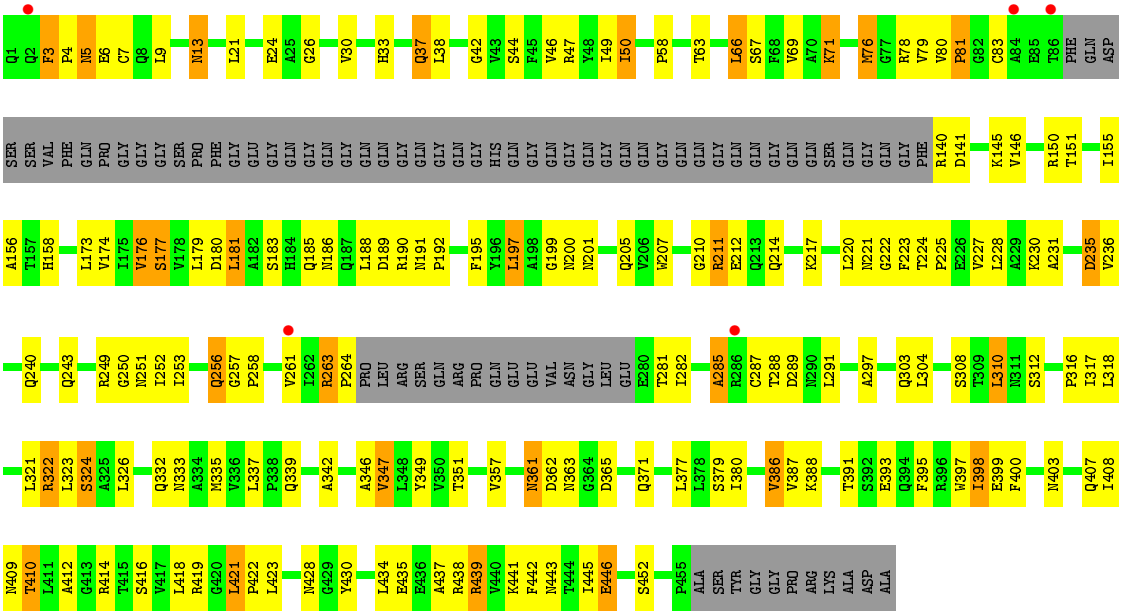






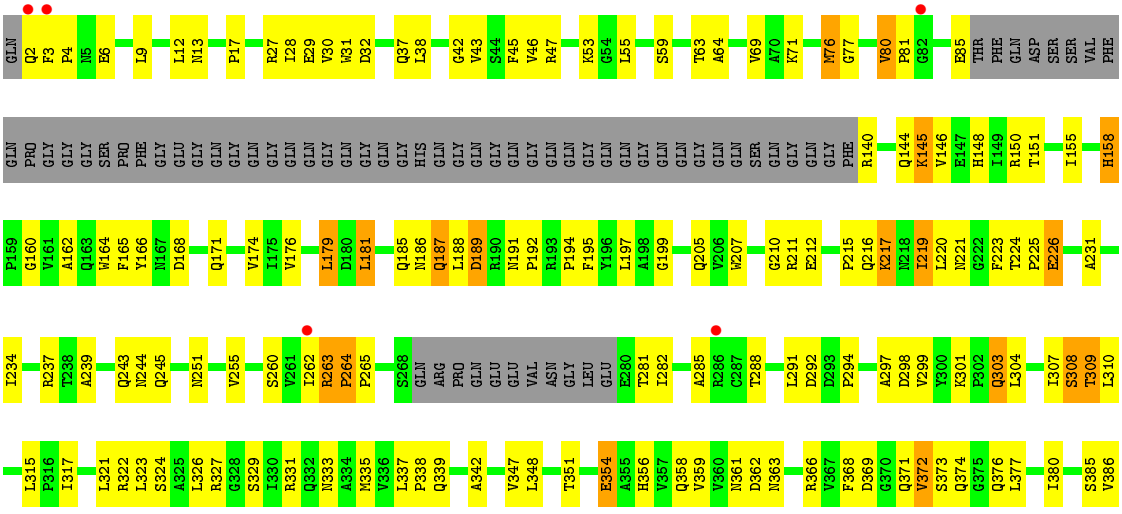
• Molecule 1: Cruciferin

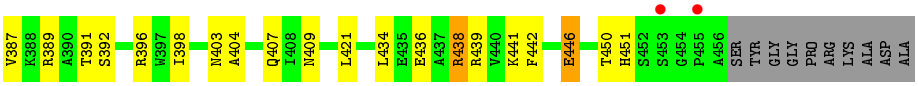
Chain C:



• Molecule 1: Cruciferin

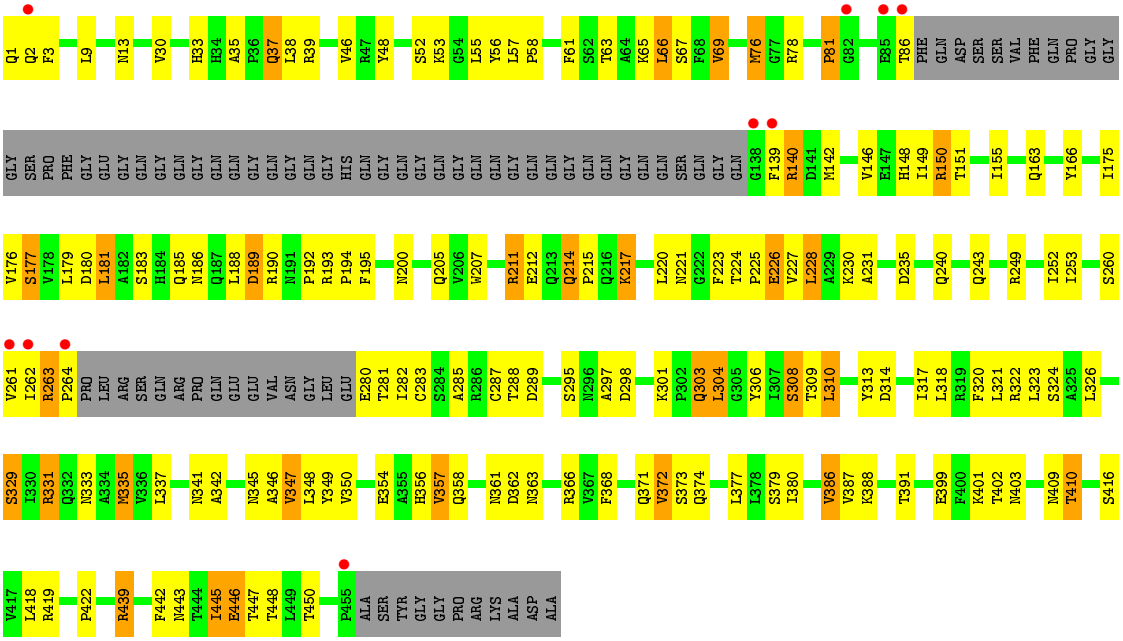
Chain D:





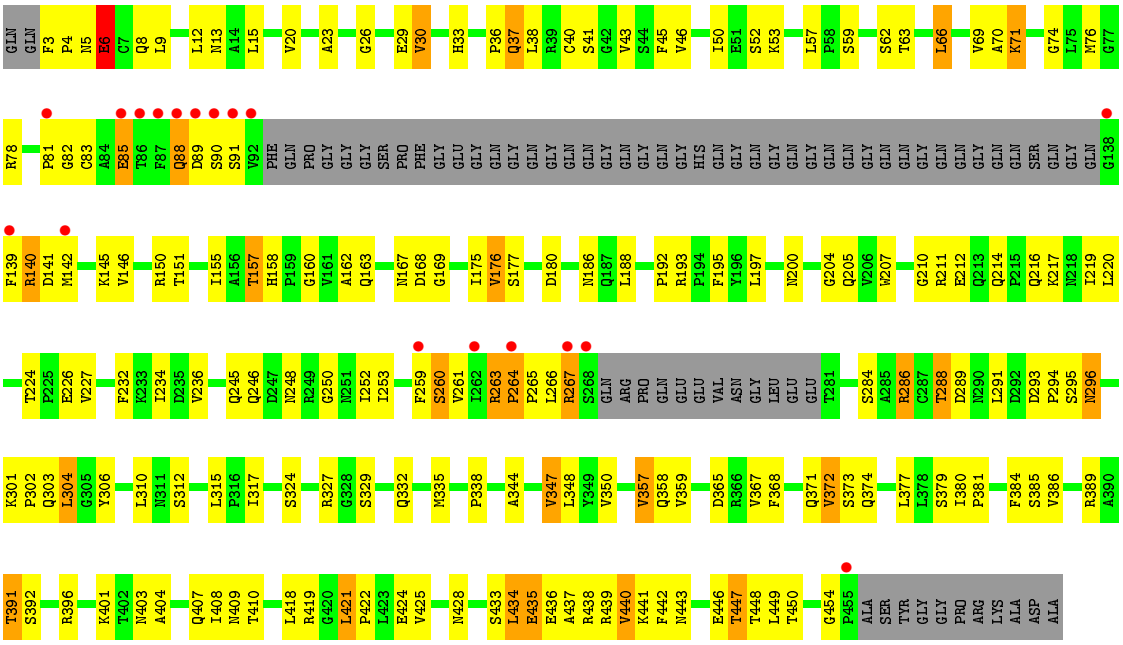
- Molecule 1: Cruciferin

Chain E:



- Molecule 1: Cruciferin

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.10Å 190.41Å 99.90Å 90.00° 114.00° 90.00°	Depositor
Resolution (Å)	49.79 – 2.98 49.79 – 2.98	Depositor EDS
% Data completeness (in resolution range)	94.4 (49.79-2.98) 94.4 (49.79-2.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.158 , 0.250 0.147 , 0.242	Depositor DCC
R_{free} test set	3287 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.7	EDS
Estimated twinning fraction	0.459 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 65651 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18711	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 3.88% 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, 0.375 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: GOL, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.42	0/3200	0.59	0/4346
1	B	0.43	0/3105	0.61	0/4218
1	C	0.41	0/3108	0.61	0/4221
1	D	0.43	0/3130	0.60	0/4251
1	E	0.42	0/3124	0.61	0/4242
1	F	0.41	0/3187	0.60	0/4329
All	All	0.42	0/18854	0.60	0/25607

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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	LEU	Peptide
1	C	188	LEU	Peptide

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	3134	0	3079	171	0
1	B	3042	0	2995	164	0
1	C	3046	0	2998	156	0
1	D	3067	0	3021	138	0
1	E	3061	0	3010	145	0
1	F	3119	0	3069	155	0
2	A	6	0	8	1	0
2	B	6	0	8	1	0
2	C	6	0	8	1	0
2	D	6	0	8	4	0
2	E	6	0	8	4	0
2	F	6	0	8	1	0
3	A	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	F	5	0	0	0	0
4	A	29	0	0	1	0
4	B	37	0	0	1	0
4	C	25	0	0	1	0
4	D	44	0	0	1	0
4	E	27	0	0	0	0
4	F	24	0	0	1	0
All	All	18711	0	18220	827	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 (827) 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:A:329:SER:OG	1:A:396:ARG:HD2	1.53	1.06
1:D:359:VAL:HG22	1:D:386:VAL:HG22	1.43	1.00
1:C:37:GLN:HG3	1:C:379:SER:HB3	1.45	0.96
1:C:361:ASN:HB3	1:C:363:ASN:H	1.34	0.93
1:F:13:ASN:H	1:F:37:GLN:HE22	1.19	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:ILE:HD13	1:F:386:VAL:HG21	1.55	0.89
1:C:439:ARG:HH11	1:C:439:ARG:HG3	1.38	0.88
1:E:356:HIS:HB2	1:E:371:GLN:HE22	1.39	0.87
1:D:291:LEU:HD22	1:D:308:SER:HB3	1.56	0.87
1:D:263:ARG:N	1:D:264:PRO:HD3	1.89	0.87
1:A:263:ARG:HB2	1:A:264:PRO:HD3	1.54	0.87
1:B:237:ARG:HD2	1:B:237:ARG:H	1.37	0.87
1:A:184:HIS:HD2	1:A:322:ARG:HH11	1.19	0.87
1:A:347:VAL:HG13	1:A:377:LEU:HD11	1.57	0.87
1:E:193:ARG:HH22	1:F:8:GLN:NE2	1.73	0.87
1:A:217:LYS:H	1:A:217:LYS:HD2	1.38	0.86
1:F:205:GLN:HB2	1:F:211:ARG:HG3	1.58	0.85
1:A:260:SER:HB2	1:A:263:ARG:HD3	1.57	0.85
1:D:347:VAL:HG12	1:D:377:LEU:HD11	1.60	0.84
1:E:280:GLU:HG3	1:E:281:THR:H	1.42	0.84
1:B:282:ILE:HB	1:B:285:ALA:HB2	1.60	0.84
1:D:329:SER:OG	1:D:396:ARG:HD2	1.77	0.83
1:F:347:VAL:HG13	1:F:377:LEU:HD11	1.61	0.82
1:D:373:SER:O	1:D:376:GLN:HG3	1.79	0.82
1:A:350:VAL:HG21	1:A:372:VAL:HG12	1.61	0.82
1:A:294:PRO:HB3	1:A:300:TYR:CE1	2.16	0.81
1:E:194:PRO:HG3	2:E:467:GOL:H11	1.60	0.81
1:C:371:GLN:HE22	1:C:391:THR:HG21	1.45	0.81
1:F:446:GLU:HG3	1:F:450:THR:HB	1.63	0.80
1:B:351:THR:O	1:B:374:GLN:HG3	1.82	0.80
1:C:410:THR:HG22	1:C:416:SER:HA	1.62	0.80
1:D:148:HIS:HE1	1:D:264:PRO:HG2	1.45	0.80
1:F:263:ARG:NE	1:F:263:ARG:HA	1.98	0.79
1:C:221:ASN:HA	1:C:243:GLN:HG2	1.65	0.79
1:E:140:ARG:HG3	1:E:140:ARG:HH11	1.45	0.79
1:B:77:GLY:HA3	1:B:164:TRP:CE2	2.18	0.79
1:C:439:ARG:NH1	1:C:439:ARG:HG3	1.93	0.79
1:F:20:VAL:HG22	1:F:29:GLU:HG2	1.64	0.79
1:D:160:GLY:HA3	1:E:342:ALA:HB1	1.65	0.79
1:B:263:ARG:O	1:B:265:PRO:HD3	1.83	0.78
1:F:37:GLN:HG3	1:F:379:SER:HB3	1.65	0.78
1:C:214:GLN:HE21	1:E:13:ASN:HD21	1.31	0.78
1:F:286:ARG:HB3	1:F:286:ARG:HH11	1.48	0.77
1:C:67:SER:HA	1:C:177:SER:HB3	1.67	0.77
1:B:302:PRO:HD2	4:B:1123:HOH:O	1.84	0.77
1:F:436:GLU:O	1:F:440:VAL:HG12	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:SER:HB3	1:F:263:ARG:HD3	1.66	0.77
1:F:155:ILE:HG13	1:F:288:THR:HG23	1.67	0.76
1:E:419:ARG:NH1	1:E:442:PHE:HA	2.00	0.76
1:D:371:GLN:HG2	4:D:1110:HOH:O	1.84	0.76
1:C:37:GLN:HB3	1:E:212:GLU:OE2	1.85	0.76
1:D:146:VAL:HG12	1:D:262:ILE:HD11	1.66	0.76
1:A:92:VAL:HG23	1:A:93:PHE:H	1.48	0.76
1:E:139:PHE:HB2	1:E:263:ARG:HE	1.50	0.75
1:D:69:VAL:HG22	1:D:151:THR:HA	1.68	0.75
1:B:3:PHE:CD2	1:B:4:PRO:HA	2.21	0.75
1:E:183:SER:OG	1:E:185:GLN:HG3	1.86	0.74
1:A:446:GLU:HG3	1:A:450:THR:HB	1.68	0.74
1:E:188:LEU:HD23	1:E:193:ARG:HD2	1.69	0.74
1:F:267:ARG:HH21	1:F:267:ARG:HB2	1.52	0.74
1:A:263:ARG:CB	1:A:264:PRO:HD3	2.17	0.74
1:F:433:SER:HB2	1:F:436:GLU:H	1.51	0.73
1:E:356:HIS:HB2	1:E:371:GLN:NE2	2.03	0.73
1:A:87:PHE:HE2	1:A:145:LYS:HE2	1.52	0.73
1:F:267:ARG:HH21	1:F:267:ARG:CB	2.02	0.73
1:B:22:LYS:H	1:B:203:GLN:HE22	1.37	0.73
1:F:263:ARG:HE	1:F:263:ARG:HA	1.52	0.72
1:F:350:VAL:HG21	1:F:372:VAL:HG13	1.70	0.72
1:F:69:VAL:HG21	1:F:150:ARG:O	1.89	0.72
1:E:211:ARG:HE	1:E:211:ARG:HA	1.53	0.72
1:A:69:VAL:HG21	1:A:150:ARG:O	1.89	0.72
1:F:357:VAL:HG22	1:F:368:PHE:CE2	2.25	0.71
1:A:20:VAL:HG22	1:A:29:GLU:HG2	1.72	0.71
1:B:205:GLN:HB2	1:B:211:ARG:HG3	1.71	0.71
1:A:292:ASP:O	1:A:294:PRO:HD3	1.90	0.71
1:B:3:PHE:CG	1:B:4:PRO:HA	2.25	0.71
1:D:148:HIS:CE1	1:D:264:PRO:HG2	2.26	0.71
1:F:263:ARG:HB2	1:F:264:PRO:HD3	1.72	0.71
1:A:89:ASP:HB2	1:A:141:ASP:HB3	1.71	0.71
1:D:409:ASN:OD1	1:F:81:PRO:HG3	1.91	0.71
1:A:324:SER:HB2	1:A:403:ASN:O	1.90	0.71
1:B:210:GLY:HA2	1:F:36:PRO:HD3	1.73	0.71
1:C:423:LEU:HD22	1:C:437:ALA:HB1	1.73	0.70
1:D:335:MET:CE	1:D:337:LEU:HD23	2.21	0.70
1:A:217:LYS:N	1:A:217:LYS:HD2	2.06	0.70
1:C:282:ILE:CG2	1:C:285:ALA:HB3	2.22	0.69
1:D:145:LYS:HB2	1:D:145:LYS:NZ	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:SER:HB2	1:B:403:ASN:O	1.93	0.69
1:D:362:ASP:HB3	1:F:195:PHE:CZ	2.27	0.69
1:F:266:LEU:HD12	1:F:266:LEU:O	1.93	0.69
1:B:69:VAL:HG22	1:B:151:THR:HA	1.74	0.69
1:B:235:ASP:HB3	1:B:237:ARG:HD2	1.75	0.69
1:A:211:ARG:HD2	1:B:8:GLN:HE22	1.58	0.69
1:A:160:GLY:HA3	1:B:342:ALA:HB1	1.75	0.69
1:C:46:VAL:HG21	2:C:467:GOL:H2	1.74	0.69
1:A:329:SER:HG	1:A:396:ARG:HD2	1.58	0.69
1:D:262:ILE:HG22	1:D:263:ARG:H	1.58	0.68
1:A:407:GLN:HE21	1:C:81:PRO:HB2	1.57	0.68
1:C:140:ARG:N	1:C:263:ARG:HH11	1.92	0.68
1:E:205:GLN:OE1	1:E:211:ARG:HD3	1.93	0.68
1:B:267:ARG:HH21	1:B:267:ARG:HB2	1.58	0.68
1:F:195:PHE:HB3	1:F:219:ILE:HD11	1.75	0.68
1:A:282:ILE:CG2	1:A:285:ALA:HB2	2.23	0.68
1:B:224:THR:OG1	1:B:227:VAL:HG12	1.92	0.68
1:E:63:THR:HG21	1:E:181:LEU:HD12	1.75	0.68
1:E:2:GLN:HG2	1:E:39:ARG:NH2	2.09	0.68
1:F:286:ARG:HH11	1:F:286:ARG:CG	2.06	0.68
1:A:63:THR:HG22	1:A:186:ASN:HB2	1.73	0.68
1:B:211:ARG:NE	1:B:211:ARG:HA	2.09	0.68
1:A:1:GLN:HE22	1:C:210:GLY:HA3	1.58	0.68
1:E:65:LYS:HG2	1:E:179:LEU:HD23	1.75	0.67
1:B:237:ARG:CD	1:B:237:ARG:H	2.05	0.67
1:B:259:PHE:CE2	1:B:261:VAL:HG21	2.29	0.67
1:E:301:LYS:HE2	1:E:304:LEU:HD23	1.74	0.67
1:B:12:LEU:HB2	1:B:368:PHE:HB2	1.77	0.67
1:E:215:PRO:O	1:E:217:LYS:HE3	1.94	0.67
1:A:184:HIS:CD2	1:A:322:ARG:HH11	2.08	0.67
1:F:286:ARG:HH11	1:F:286:ARG:CB	2.07	0.67
1:E:410:THR:HG22	1:E:416:SER:HA	1.76	0.67
1:A:371:GLN:NE2	1:A:391:THR:HG21	2.10	0.67
1:C:347:VAL:HG13	1:C:377:LEU:HD11	1.76	0.67
1:A:80:VAL:HG21	1:A:83:CYS:SG	2.35	0.67
1:D:3:PHE:CD1	1:D:4:PRO:HA	2.30	0.67
1:F:419:ARG:O	1:F:441:LYS:HE3	1.95	0.67
1:A:188:LEU:HD13	1:B:382:GLN:HB3	1.77	0.67
1:F:188:LEU:HD23	1:F:193:ARG:HD2	1.76	0.67
1:C:69:VAL:HG23	1:C:151:THR:HA	1.75	0.67
1:C:263:ARG:HB2	1:C:264:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:VAL:HG21	2:B:467:GOL:H2	1.75	0.66
1:C:141:ASP:O	1:C:264:PRO:HG3	1.95	0.66
1:D:187:GLN:NE2	1:E:402:THR:OG1	2.29	0.66
1:A:217:LYS:CD	1:A:217:LYS:H	2.09	0.66
1:C:199:GLY:HA3	1:C:251:ASN:HD22	1.59	0.66
1:A:139:PHE:CZ	1:B:438:ARG:HG3	2.30	0.66
1:C:282:ILE:HG21	1:C:285:ALA:HB3	1.78	0.66
1:A:330:ILE:HG13	1:A:390:ALA:HB2	1.78	0.66
1:E:263:ARG:HB2	1:E:264:PRO:HA	1.77	0.66
1:E:86:THR:HG21	1:E:264:PRO:HB2	1.77	0.66
1:A:195:PHE:CZ	1:B:362:ASP:HB3	2.31	0.66
1:C:69:VAL:HG21	1:C:150:ARG:O	1.96	0.66
1:A:13:ASN:H	1:A:37:GLN:HE22	1.40	0.66
1:B:263:ARG:H	1:B:263:ARG:HD2	1.61	0.66
1:A:211:ARG:HA	1:A:211:ARG:HE	1.59	0.66
1:A:45:PHE:CZ	1:A:176:VAL:HG13	2.31	0.66
1:D:362:ASP:HB3	1:F:195:PHE:CE1	2.31	0.65
1:F:357:VAL:HG22	1:F:368:PHE:HE2	1.60	0.65
1:A:380:ILE:HD13	1:A:386:VAL:HG21	1.76	0.65
1:F:3:PHE:HA	1:F:5:ASN:H	1.61	0.65
1:E:230:LYS:NZ	1:F:454:GLY:HA2	2.12	0.65
1:F:3:PHE:CG	1:F:4:PRO:HA	2.31	0.65
1:B:205:GLN:HA	1:B:207:TRP:CZ3	2.32	0.65
1:C:66:LEU:HB2	1:C:323:LEU:HD13	1.78	0.65
1:A:81:PRO:HG3	1:B:409:ASN:OD1	1.96	0.65
1:C:326:LEU:C	1:C:326:LEU:HD23	2.17	0.65
1:C:361:ASN:HB3	1:C:363:ASN:N	2.10	0.65
1:D:195:PHE:HD1	1:D:219:ILE:HD11	1.61	0.64
1:A:212:GLU:OE1	1:D:37:GLN:NE2	2.30	0.64
1:A:90:SER:HB2	1:A:263:ARG:HG3	1.79	0.64
1:B:231:ALA:HB2	1:C:335:MET:HE3	1.79	0.64
1:A:194:PRO:HD2	4:A:686:HOH:O	1.97	0.64
1:D:77:GLY:HA3	1:D:164:TRP:CE2	2.31	0.64
1:B:265:PRO:HB3	1:B:267:ARG:HD3	1.80	0.64
1:F:447:THR:HG22	1:F:448:THR:N	2.13	0.64
1:B:37:GLN:NE2	1:F:212:GLU:OE1	2.31	0.64
1:B:255:VAL:HG13	1:C:428:ASN:ND2	2.14	0.63
1:D:335:MET:HE2	1:D:337:LEU:HD23	1.80	0.63
1:A:146:VAL:HG21	1:A:261:VAL:CG1	2.28	0.63
1:C:421:LEU:O	1:C:441:LYS:HE3	1.98	0.63
1:B:11:GLN:HE22	1:F:214:GLN:HE22	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HD3	1:B:362:ASP:OD2	1.99	0.62
1:A:1:GLN:HA	1:E:1:GLN:HG2	1.81	0.62
1:F:45:PHE:CE2	1:F:176:VAL:HG22	2.34	0.62
1:A:139:PHE:HD1	1:A:140:ARG:O	1.82	0.62
1:E:78:ARG:CZ	1:E:287:CYS:HB2	2.30	0.62
1:B:380:ILE:HD13	1:B:386:VAL:HG21	1.80	0.62
1:A:419:ARG:O	1:A:441:LYS:HE3	1.99	0.62
1:C:326:LEU:O	1:C:398:ILE:HD13	1.99	0.62
1:E:439:ARG:HB2	1:E:443:ASN:OD1	1.99	0.62
1:C:256:GLN:HA	1:C:256:GLN:NE2	2.13	0.62
1:E:227:VAL:HG11	1:F:358:GLN:NE2	2.14	0.62
1:F:267:ARG:HH21	1:F:267:ARG:CG	2.11	0.62
1:D:194:PRO:HG3	2:D:467:GOL:H32	1.82	0.62
1:D:262:ILE:C	1:D:264:PRO:HD3	2.19	0.61
1:F:13:ASN:H	1:F:37:GLN:NE2	1.95	0.61
1:E:81:PRO:HB3	1:F:409:ASN:OD1	2.00	0.61
1:B:366:ARG:HD3	1:B:369:ASP:HB2	1.82	0.61
1:B:347:VAL:HG22	1:B:377:LEU:HD11	1.82	0.61
1:B:59:SER:O	1:B:162:ALA:HA	2.00	0.61
1:B:338:PRO:HA	1:B:386:VAL:O	2.00	0.61
1:B:359:VAL:HG22	1:B:386:VAL:HG22	1.83	0.61
1:C:185:GLN:HE22	1:C:321:LEU:HA	1.65	0.61
1:F:85:GLU:HG2	1:F:142:MET:HB2	1.81	0.61
1:B:351:THR:HB	1:B:396:ARG:O	2.01	0.61
1:D:195:PHE:CZ	1:E:362:ASP:HB3	2.36	0.61
1:B:332:GLN:HB2	1:B:392:SER:O	2.01	0.61
1:B:199:GLY:HA3	1:B:251:ASN:HD22	1.65	0.61
1:E:146:VAL:HG21	1:E:261:VAL:HG13	1.82	0.61
1:E:446:GLU:HG3	1:E:450:THR:HB	1.83	0.61
1:E:282:ILE:HG21	1:E:285:ALA:HB2	1.81	0.61
1:F:146:VAL:HG21	1:F:261:VAL:CG1	2.31	0.61
1:B:29:GLU:OE1	1:B:47:ARG:NH1	2.33	0.61
1:B:223:PHE:HE1	1:C:387:VAL:HG12	1.66	0.60
1:F:63:THR:HG22	1:F:186:ASN:HB2	1.82	0.60
1:A:74:GLY:HA2	1:A:168:ASP:OD1	2.01	0.60
1:F:9:LEU:HD21	1:F:37:GLN:HA	1.83	0.60
1:F:13:ASN:N	1:F:37:GLN:HE22	1.93	0.60
1:D:354:GLU:HG2	1:D:392:SER:HB3	1.83	0.60
1:B:210:GLY:HA2	1:F:36:PRO:CD	2.32	0.60
1:F:89:ASP:HB2	1:F:141:ASP:HB3	1.83	0.60
1:D:231:ALA:HA	1:E:335:MET:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ARG:NH1	1:C:442:PHE:HA	2.17	0.60
1:E:347:VAL:HG13	1:E:377:LEU:HD11	1.84	0.60
1:A:263:ARG:HB2	1:A:264:PRO:CD	2.30	0.60
1:C:37:GLN:CG	1:C:379:SER:HB3	2.28	0.59
1:C:322:ARG:HD3	4:C:1037:HOH:O	2.02	0.59
1:B:436:GLU:O	1:B:440:VAL:HG13	2.02	0.59
1:C:180:ASP:OD2	1:C:183:SER:HB2	2.01	0.59
1:A:423:LEU:HD12	1:C:141:ASP:CG	2.22	0.59
1:A:93:PHE:O	1:A:95:PRO:HD3	2.03	0.59
1:D:185:GLN:HE22	1:D:321:LEU:HA	1.68	0.59
1:B:423:LEU:HD13	1:B:434:LEU:CD1	2.32	0.59
1:C:439:ARG:HH11	1:C:439:ARG:CG	2.12	0.59
1:F:200:ASN:O	1:F:250:GLY:HA2	2.03	0.59
1:C:337:LEU:HD13	1:C:412:ALA:O	2.03	0.58
1:C:176:VAL:HG21	1:C:349:TYR:CE2	2.38	0.58
1:A:294:PRO:HB3	1:A:300:TYR:HE1	1.66	0.58
1:C:78:ARG:NH2	1:C:287:CYS:HB2	2.18	0.58
1:D:323:LEU:O	1:D:404:ALA:HA	2.03	0.58
1:D:199:GLY:HA3	1:D:251:ASN:HD22	1.66	0.58
1:E:211:ARG:NH1	1:F:8:GLN:OE1	2.37	0.58
1:B:339:GLN:O	1:B:385:SER:HA	2.03	0.58
1:C:5:ASN:N	1:C:5:ASN:HD22	2.01	0.58
1:A:1:GLN:HG2	1:E:1:GLN:HA	1.85	0.58
1:C:183:SER:OG	1:C:185:GLN:HG3	2.04	0.58
1:F:3:PHE:CD1	1:F:4:PRO:HA	2.38	0.58
1:B:205:GLN:O	1:B:211:ARG:HG3	2.03	0.58
1:F:6:GLU:O	1:F:40:CYS:HB2	2.04	0.58
1:E:140:ARG:HG3	1:E:140:ARG:NH1	2.19	0.57
1:B:361:ASN:C	1:B:361:ASN:HD22	2.07	0.57
1:D:158:HIS:HE1	1:D:317:ILE:HD11	1.69	0.57
1:F:3:PHE:CA	1:F:5:ASN:H	2.17	0.57
1:D:194:PRO:CG	2:D:467:GOL:H32	2.35	0.57
1:B:184:HIS:HD2	1:B:322:ARG:HH21	1.53	0.57
1:B:179:LEU:HD13	1:B:192:PRO:HB3	1.86	0.57
1:F:74:GLY:HA2	1:F:168:ASP:OD1	2.04	0.57
1:E:194:PRO:CG	2:E:467:GOL:H11	2.34	0.57
1:E:326:LEU:HB3	1:E:399:GLU:HB2	1.86	0.57
1:D:434:LEU:HD22	1:D:434:LEU:H	1.70	0.57
1:F:424:GLU:O	1:F:428:ASN:ND2	2.35	0.57
1:A:371:GLN:HE21	1:A:391:THR:HG21	1.68	0.57
1:B:157:THR:HG22	1:B:161:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:LEU:HB2	1:E:323:LEU:HD13	1.87	0.57
1:C:69:VAL:O	1:C:69:VAL:HG23	2.04	0.57
1:B:373:SER:O	1:B:376:GLN:HB2	2.04	0.56
1:F:263:ARG:CB	1:F:264:PRO:HD3	2.35	0.56
1:E:282:ILE:CG2	1:E:285:ALA:HB2	2.35	0.56
1:D:199:GLY:HA3	1:D:251:ASN:ND2	2.19	0.56
1:B:157:THR:CG2	1:B:161:VAL:HB	2.35	0.56
1:D:179:LEU:HD13	1:D:192:PRO:HB3	1.87	0.56
1:B:346:ALA:HB3	1:B:380:ILE:HB	1.87	0.56
1:A:183:SER:OG	1:A:185:GLN:HG3	2.05	0.56
1:E:445:ILE:HG12	1:E:445:ILE:O	2.05	0.56
1:A:194:PRO:HG3	2:A:467:GOL:H2	1.86	0.56
1:F:204:GLY:HA2	1:F:216:GLN:HB2	1.87	0.56
1:E:321:LEU:HD12	1:E:321:LEU:H	1.70	0.56
1:D:69:VAL:CG2	1:D:151:THR:HA	2.34	0.56
1:D:347:VAL:CG1	1:D:377:LEU:HD11	2.34	0.56
1:F:3:PHE:HA	1:F:5:ASN:N	2.19	0.56
1:F:422:PRO:HB2	1:F:425:VAL:HG23	1.88	0.56
1:F:167:ASN:ND2	1:F:169:GLY:H	2.03	0.56
1:B:262:ILE:HD13	1:B:263:ARG:HH11	1.71	0.56
1:B:267:ARG:HH21	1:B:267:ARG:CB	2.18	0.56
1:F:347:VAL:CG1	1:F:377:LEU:HD11	2.34	0.55
1:E:140:ARG:H	1:E:140:ARG:HD3	1.71	0.55
1:A:37:GLN:NE2	1:D:212:GLU:OE1	2.39	0.55
1:B:230:LYS:HE3	1:C:452:SER:C	2.26	0.55
1:D:29:GLU:OE1	1:D:47:ARG:NH1	2.39	0.55
1:A:306:TYR:CE2	1:A:329:SER:HB2	2.41	0.55
1:B:335:MET:HE2	1:B:337:LEU:HA	1.87	0.55
1:B:236:VAL:O	1:B:240:GLN:HG3	2.06	0.55
1:B:335:MET:CE	1:B:338:PRO:HD3	2.37	0.55
1:E:176:VAL:HG21	1:E:349:TYR:CE2	2.41	0.55
1:E:263:ARG:HB2	1:E:264:PRO:CA	2.36	0.55
1:C:324:SER:HB3	1:C:403:ASN:O	2.06	0.55
1:B:351:THR:HG22	1:B:352:ASP:OD2	2.06	0.55
1:C:205:GLN:HB2	1:C:211:ARG:HG2	1.87	0.55
1:E:58:PRO:HA	1:E:163:GLN:O	2.06	0.55
1:F:224:THR:OG1	1:F:227:VAL:HG12	2.07	0.55
1:A:205:GLN:HB2	1:A:211:ARG:HG3	1.89	0.55
1:C:24:GLU:OE2	1:C:249:ARG:HG2	2.06	0.55
1:C:50:ILE:HB	1:C:173:LEU:HB3	1.89	0.55
1:A:89:ASP:O	1:A:140:ARG:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ASN:HB2	1:C:365:ASP:H	1.72	0.55
1:B:22:LYS:HE3	1:B:27:ARG:HD3	1.89	0.55
1:C:21:LEU:HD11	1:C:207:TRP:CZ3	2.42	0.54
1:C:249:ARG:HB3	1:C:253:ILE:HG22	1.88	0.54
1:C:211:ARG:HA	1:C:211:ARG:NE	2.22	0.54
1:A:155:ILE:HG13	1:A:288:THR:HG23	1.89	0.54
1:E:81:PRO:HB3	1:F:409:ASN:CG	2.28	0.54
1:D:262:ILE:HB	1:D:264:PRO:HD3	1.89	0.54
1:B:292:ASP:O	1:B:294:PRO:HD3	2.08	0.54
1:D:3:PHE:CG	1:D:4:PRO:HA	2.43	0.54
1:D:205:GLN:HA	1:D:207:TRP:CZ3	2.43	0.54
1:A:326:LEU:C	1:A:326:LEU:HD23	2.27	0.54
1:C:281:THR:O	1:C:282:ILE:HD13	2.08	0.54
1:A:37:GLN:HG3	1:A:379:SER:HB3	1.89	0.54
1:B:184:HIS:CD2	1:B:322:ARG:HH21	2.26	0.54
1:A:380:ILE:HG21	1:A:386:VAL:HG21	1.90	0.54
1:D:450:THR:HG23	1:D:451:HIS:O	2.08	0.54
1:E:180:ASP:OD2	1:E:183:SER:HB2	2.08	0.53
1:E:280:GLU:HG3	1:E:281:THR:N	2.20	0.53
1:D:195:PHE:CD1	1:D:219:ILE:HD11	2.43	0.53
1:B:446:GLU:HG3	1:B:450:THR:HB	1.88	0.53
1:C:37:GLN:HG3	1:C:379:SER:CB	2.30	0.53
1:C:67:SER:CA	1:C:177:SER:HB3	2.38	0.53
1:B:205:GLN:HB2	1:B:211:ARG:CG	2.35	0.53
1:A:205:GLN:NE2	1:A:211:ARG:HH11	2.07	0.53
1:F:312:SER:HB3	1:F:404:ALA:HB1	1.89	0.53
1:B:296:ASN:OD1	1:B:296:ASN:N	2.40	0.53
1:D:342:ALA:HB3	1:D:407:GLN:HB3	1.89	0.53
1:C:224:THR:O	1:C:227:VAL:HG12	2.08	0.53
1:B:195:PHE:CE1	1:C:362:ASP:HB3	2.44	0.53
1:F:52:SER:O	1:F:53:LYS:HB2	2.07	0.53
1:F:78:ARG:CG	1:F:163:GLN:HE21	2.21	0.53
1:A:80:VAL:CG2	1:A:83:CYS:SG	2.96	0.53
1:B:223:PHE:CE1	1:C:387:VAL:HG12	2.43	0.53
1:A:350:VAL:CG2	1:A:372:VAL:HG12	2.34	0.53
1:F:69:VAL:HG23	1:F:69:VAL:O	2.09	0.53
1:B:11:GLN:NE2	1:F:214:GLN:HE22	2.06	0.53
1:D:28:ILE:HG21	2:D:467:GOL:H2	1.90	0.53
1:C:78:ARG:CZ	1:C:287:CYS:HB2	2.39	0.53
1:F:332:GLN:HB2	1:F:392:SER:O	2.08	0.53
1:B:71:LYS:HB2	1:B:174:VAL:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:VAL:HG21	1:E:261:VAL:CG1	2.39	0.53
1:C:212:GLU:OE2	1:E:35:ALA:HB1	2.07	0.53
1:A:52:SER:O	1:A:53:LYS:HB2	2.09	0.53
1:E:69:VAL:HG12	1:E:175:ILE:HG12	1.90	0.52
1:B:85:GLU:HG3	1:B:144:GLN:HG3	1.89	0.52
1:F:286:ARG:HG2	1:F:286:ARG:HH11	1.72	0.52
1:A:224:THR:OG1	1:A:227:VAL:HG12	2.09	0.52
1:F:259:PHE:CE2	1:F:261:VAL:HG21	2.44	0.52
1:F:46:VAL:HG11	2:F:467:GOL:O2	2.09	0.52
1:B:369:ASP:C	1:B:369:ASP:OD2	2.48	0.52
1:A:381:PRO:HD2	1:A:384:PHE:CD2	2.44	0.52
1:C:221:ASN:HA	1:C:243:GLN:CG	2.38	0.52
1:B:423:LEU:HD13	1:B:434:LEU:HD12	1.90	0.52
1:B:195:PHE:CZ	1:C:362:ASP:HB3	2.44	0.52
1:A:433:SER:HB2	1:A:436:GLU:H	1.73	0.52
1:F:91:SER:HA	1:F:263:ARG:NH2	2.25	0.52
1:A:87:PHE:CD1	1:A:262:ILE:HG23	2.45	0.52
1:E:249:ARG:HB3	1:E:253:ILE:HG22	1.90	0.52
1:A:217:LYS:CD	1:A:217:LYS:N	2.70	0.52
1:A:282:ILE:HG21	1:A:285:ALA:HB2	1.90	0.52
1:E:33:HIS:CE1	1:E:192:PRO:HD2	2.45	0.52
1:B:235:ASP:HB3	1:B:237:ARG:CD	2.39	0.52
1:A:259:PHE:CE2	1:A:261:VAL:HG21	2.45	0.52
1:B:184:HIS:HD2	1:B:322:ARG:NH2	2.07	0.52
1:F:439:ARG:HG2	1:F:443:ASN:OD1	2.10	0.52
1:F:433:SER:HB3	1:F:435:GLU:HG2	1.91	0.52
1:A:200:ASN:O	1:A:250:GLY:HA2	2.10	0.51
1:C:380:ILE:HD13	1:C:386:VAL:HG21	1.91	0.51
1:D:366:ARG:CD	1:D:369:ASP:HB2	2.40	0.51
1:B:414:ARG:HA	1:B:419:ARG:NH1	2.25	0.51
1:A:216:GLN:HG3	1:B:363:ASN:HA	1.93	0.51
1:E:324:SER:HB2	1:E:403:ASN:O	2.09	0.51
1:E:211:ARG:HA	1:E:211:ARG:NE	2.24	0.51
1:A:335:MET:HE3	1:C:231:ALA:HA	1.92	0.51
1:C:263:ARG:CZ	1:C:263:ARG:HB3	2.39	0.51
1:D:223:PHE:HE1	1:E:387:VAL:HG12	1.76	0.51
1:B:81:PRO:HG2	1:C:407:GLN:HG3	1.91	0.51
1:B:211:ARG:HE	1:B:211:ARG:HA	1.74	0.51
1:A:324:SER:CB	1:A:403:ASN:O	2.57	0.51
1:D:264:PRO:CB	1:D:265:PRO:HA	2.39	0.51
1:B:306:TYR:CE2	1:B:329:SER:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:MET:HG2	1:E:450:THR:HG23	1.92	0.51
1:B:44:SER:CB	1:B:192:PRO:HG3	2.40	0.51
1:B:81:PRO:HG3	1:C:409:ASN:ND2	2.25	0.51
1:E:231:ALA:HA	1:F:335:MET:HE3	1.93	0.51
1:F:286:ARG:HG2	1:F:286:ARG:NH1	2.26	0.51
1:C:388:LYS:HE2	1:C:399:GLU:OE2	2.10	0.51
1:D:371:GLN:HE22	1:D:391:THR:HG21	1.76	0.51
1:B:211:ARG:HE	1:B:211:ARG:CA	2.22	0.51
1:E:55:LEU:O	1:E:252:ILE:HA	2.11	0.51
1:D:12:LEU:HB2	1:D:368:PHE:HB2	1.93	0.51
1:A:348:LEU:O	1:A:377:LEU:HA	2.11	0.51
1:D:263:ARG:HH11	1:D:263:ARG:HB3	1.76	0.51
1:E:37:GLN:HG3	1:E:379:SER:CB	2.41	0.50
1:B:66:LEU:HD12	1:B:323:LEU:HB3	1.92	0.50
1:D:441:LYS:HD3	1:D:442:PHE:CE2	2.46	0.50
1:F:71:LYS:HA	1:F:151:THR:OG1	2.11	0.50
1:C:439:ARG:HA	1:C:443:ASN:ND2	2.26	0.50
1:E:185:GLN:NE2	1:E:320:PHE:O	2.44	0.50
1:C:211:ARG:O	1:C:211:ARG:HD3	2.11	0.50
1:D:366:ARG:HD3	1:D:369:ASP:HB2	1.92	0.50
1:E:357:VAL:HG22	1:E:368:PHE:CE2	2.45	0.50
1:A:360:VAL:HG11	1:C:222:GLY:HA3	1.93	0.50
1:A:389:ARG:HD3	3:A:474:SO4:O2	2.11	0.50
1:A:300:TYR:CE2	1:A:302:PRO:HG3	2.46	0.50
1:B:3:PHE:HD2	1:B:6:GLU:HG2	1.76	0.50
1:A:141:ASP:OD1	1:B:441:LYS:NZ	2.44	0.50
1:D:434:LEU:HD22	1:D:434:LEU:N	2.27	0.50
1:E:155:ILE:HG21	1:E:163:GLN:HE22	1.76	0.50
1:E:52:SER:O	1:E:53:LYS:HB2	2.11	0.50
1:F:301:LYS:HE3	4:F:573:HOH:O	2.11	0.50
1:D:221:ASN:HA	1:D:243:GLN:HG2	1.94	0.50
1:F:50:ILE:HG23	1:F:252:ILE:CG2	2.42	0.50
1:A:90:SER:H	1:A:263:ARG:HG3	1.76	0.50
1:A:407:GLN:HE21	1:C:81:PRO:CB	2.24	0.50
1:A:423:LEU:HD12	1:C:141:ASP:OD2	2.11	0.50
1:B:335:MET:HE1	1:B:337:LEU:HD23	1.93	0.50
1:A:66:LEU:HD23	1:A:155:ILE:O	2.12	0.50
1:F:286:ARG:NH1	1:F:286:ARG:CG	2.71	0.50
1:B:231:ALA:HA	1:C:335:MET:HE1	1.93	0.50
1:C:156:ALA:HB1	1:C:321:LEU:HD21	1.94	0.50
1:E:326:LEU:HD23	1:E:326:LEU:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ALA:HA	1:C:308:SER:HB2	1.93	0.50
1:A:33:HIS:CE1	1:A:192:PRO:HD2	2.47	0.50
1:D:155:ILE:HG12	1:D:288:THR:HG23	1.93	0.50
1:B:234:ILE:HD12	1:B:238:THR:HB	1.93	0.50
1:D:282:ILE:HG22	1:D:285:ALA:H	1.77	0.50
1:C:71:LYS:HA	1:C:151:THR:OG1	2.11	0.49
1:E:225:PRO:HD2	1:E:226:GLU:OE2	2.12	0.49
1:B:36:PRO:HD2	1:F:212:GLU:OE2	2.12	0.49
1:C:418:LEU:HD12	1:C:421:LEU:HD22	1.92	0.49
1:D:438:ARG:HD2	1:F:139:PHE:CZ	2.47	0.49
1:E:350:VAL:HG21	1:E:372:VAL:HG22	1.94	0.49
1:D:80:VAL:HB	1:D:81:PRO:HD2	1.94	0.49
1:C:58:PRO:O	1:C:197:LEU:HB2	2.13	0.49
1:E:205:GLN:HB2	1:E:211:ARG:HG3	1.93	0.49
1:E:65:LYS:HG2	1:E:179:LEU:CD2	2.40	0.49
1:A:216:GLN:HG3	1:B:363:ASN:OD1	2.12	0.49
1:D:81:PRO:HD3	1:E:409:ASN:HD21	1.78	0.49
1:A:249:ARG:HB3	1:A:253:ILE:HG22	1.94	0.49
1:C:76:MET:O	1:C:76:MET:HG3	2.12	0.49
1:D:231:ALA:HB2	1:E:335:MET:HE1	1.95	0.49
1:A:69:VAL:HG23	1:A:152:GLY:H	1.78	0.49
1:E:226:GLU:O	1:E:230:LYS:HG3	2.12	0.49
1:C:347:VAL:CG1	1:C:377:LEU:HD11	2.43	0.49
1:E:146:VAL:HG11	1:E:261:VAL:HG11	1.95	0.49
1:D:292:ASP:O	1:D:294:PRO:HD3	2.12	0.49
1:F:232:PHE:HB2	1:F:234:ILE:HG12	1.95	0.49
1:A:230:LYS:HE2	1:B:453:SER:O	2.13	0.49
1:C:414:ARG:HD2	1:C:445:ILE:O	2.12	0.49
1:D:262:ILE:CB	1:D:264:PRO:HD3	2.43	0.49
1:E:320:PHE:O	1:E:322:ARG:HG3	2.13	0.49
1:D:322:ARG:HA	1:D:404:ALA:HB2	1.94	0.49
1:A:8:GLN:NE2	1:C:211:ARG:NH1	2.61	0.49
1:E:139:PHE:HB2	1:E:263:ARG:NE	2.22	0.48
1:A:91:SER:HB3	1:A:139:PHE:O	2.13	0.48
1:D:434:LEU:O	1:D:438:ARG:HB2	2.13	0.48
1:A:21:LEU:HA	1:A:203:GLN:OE1	2.12	0.48
1:D:348:LEU:C	1:D:348:LEU:HD23	2.33	0.48
1:D:224:THR:HG22	1:E:366:ARG:NH1	2.28	0.48
1:C:349:TYR:HB3	1:C:398:ILE:HG22	1.94	0.48
1:E:335:MET:CE	1:E:337:LEU:HD23	2.43	0.48
1:C:49:ILE:HD13	1:C:174:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PHE:O	1:A:234:ILE:HG23	2.12	0.48
1:B:386:VAL:HG12	1:B:387:VAL:N	2.28	0.48
1:E:81:PRO:HG2	1:F:407:GLN:HE21	1.78	0.48
1:B:41:SER:HB3	1:B:43:VAL:HG22	1.95	0.48
1:A:263:ARG:CB	1:A:264:PRO:CD	2.90	0.48
1:A:205:GLN:NE2	1:A:211:ARG:HD3	2.29	0.48
1:A:416:SER:HB3	1:A:419:ARG:HB2	1.96	0.48
1:E:348:LEU:O	1:E:377:LEU:HA	2.13	0.48
1:D:281:THR:HG22	1:E:313:TYR:OH	2.13	0.48
1:B:22:LYS:H	1:B:203:GLN:NE2	2.09	0.48
1:B:41:SER:HA	1:B:345:ASN:ND2	2.28	0.48
1:A:424:GLU:O	1:A:428:ASN:HB2	2.14	0.48
1:D:307:ILE:HG23	1:D:326:LEU:HD21	1.95	0.48
1:B:3:PHE:C	1:B:5:ASN:H	2.17	0.48
1:D:407:GLN:HG2	1:F:81:PRO:HG2	1.96	0.48
1:A:407:GLN:HG2	1:C:81:PRO:HG2	1.95	0.48
1:E:227:VAL:HG11	1:F:358:GLN:HE22	1.78	0.48
1:B:280:GLU:HB3	1:B:282:ILE:CD1	2.44	0.48
1:C:4:PRO:C	1:C:5:ASN:HD22	2.17	0.48
1:C:257:GLY:HA3	1:C:258:PRO:HD3	1.65	0.48
1:C:438:ARG:NH1	1:C:438:ARG:HB2	2.29	0.48
1:A:211:ARG:HA	1:A:211:ARG:NE	2.28	0.47
1:F:338:PRO:HA	1:F:386:VAL:O	2.14	0.47
1:F:43:VAL:HG12	1:F:180:ASP:HA	1.95	0.47
1:D:262:ILE:HG22	1:D:263:ARG:N	2.28	0.47
1:E:55:LEU:HD21	1:F:425:VAL:HG13	1.95	0.47
1:B:361:ASN:HD21	1:B:365:ASP:H	1.62	0.47
1:F:78:ARG:HD3	1:F:163:GLN:HE21	1.78	0.47
1:B:32:ASP:O	1:B:38:LEU:HD12	2.14	0.47
1:C:410:THR:HG22	1:C:416:SER:CA	2.37	0.47
1:E:318:LEU:HD22	1:E:323:LEU:O	2.15	0.47
1:F:59:SER:O	1:F:162:ALA:HA	2.14	0.47
1:F:304:LEU:HD12	1:F:304:LEU:HA	1.73	0.47
1:B:188:LEU:O	1:C:7:CYS:SG	2.72	0.47
1:C:63:THR:HG22	1:C:186:ASN:HB2	1.96	0.47
1:B:36:PRO:HD3	1:F:210:GLY:HA2	1.95	0.47
1:A:180:ASP:OD2	1:A:183:SER:HB2	2.15	0.47
1:D:372:VAL:CG1	1:D:372:VAL:O	2.63	0.47
1:C:156:ALA:HB1	1:C:321:LEU:CD2	2.44	0.47
1:C:211:ARG:O	1:C:212:GLU:HB2	2.14	0.47
1:E:221:ASN:HA	1:E:243:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:VAL:HG21	2:D:467:GOL:H12	1.97	0.47
1:D:64:ALA:HB2	1:D:185:GLN:NE2	2.30	0.47
1:E:69:VAL:HG11	1:E:149:ILE:HD12	1.95	0.47
1:F:50:ILE:HG23	1:F:252:ILE:HG21	1.97	0.47
1:E:288:THR:CG2	1:E:289:ASP:N	2.78	0.47
1:C:235:ASP:N	1:C:235:ASP:OD1	2.44	0.47
1:D:63:THR:HG22	1:D:186:ASN:HB2	1.97	0.47
1:C:38:LEU:HD23	1:C:38:LEU:HA	1.73	0.47
1:E:263:ARG:CB	1:E:264:PRO:CA	2.92	0.47
1:F:329:SER:CB	1:F:396:ARG:HD2	2.45	0.47
1:F:344:ALA:HB2	1:F:403:ASN:HB2	1.96	0.47
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.76	0.47
1:B:205:GLN:HB2	1:B:211:ARG:CD	2.45	0.47
1:F:441:LYS:HE2	1:F:442:PHE:CZ	2.50	0.47
1:E:146:VAL:HG11	1:E:261:VAL:CG1	2.45	0.47
1:E:249:ARG:NH1	1:E:253:ILE:HG21	2.30	0.47
1:F:329:SER:OG	1:F:396:ARG:HD2	2.15	0.47
1:C:179:LEU:HD13	1:C:192:PRO:HB3	1.97	0.47
1:E:200:ASN:HD22	1:E:217:LYS:HA	1.79	0.46
1:A:37:GLN:CG	1:A:379:SER:HB3	2.45	0.46
1:B:335:MET:CE	1:B:337:LEU:HD23	2.45	0.46
1:C:50:ILE:HD13	1:C:252:ILE:HD13	1.95	0.46
1:A:436:GLU:O	1:A:440:VAL:HG23	2.15	0.46
1:F:70:ALA:O	1:F:71:LYS:HB3	2.15	0.46
1:D:294:PRO:HA	1:D:297:ALA:HB2	1.96	0.46
1:A:90:SER:N	1:A:263:ARG:HG3	2.30	0.46
1:F:264:PRO:O	1:F:266:LEU:N	2.45	0.46
1:B:259:PHE:CZ	1:B:261:VAL:HG21	2.50	0.46
1:A:20:VAL:CG2	1:A:29:GLU:HG2	2.43	0.46
1:B:361:ASN:ND2	1:B:365:ASP:H	2.12	0.46
1:D:59:SER:O	1:D:162:ALA:HA	2.14	0.46
1:B:64:ALA:HB2	1:B:185:GLN:NE2	2.31	0.46
1:D:338:PRO:HA	1:D:386:VAL:O	2.15	0.46
1:C:26:GLY:HA3	1:C:49:ILE:O	2.16	0.46
1:E:306:TYR:CE2	1:E:329:SER:HB3	2.51	0.46
1:B:433:SER:HB3	1:B:436:GLU:HG3	1.97	0.46
1:C:44:SER:HB3	1:C:179:LEU:HD12	1.97	0.46
1:F:291:LEU:HB3	1:F:327:ARG:HB3	1.97	0.46
1:A:304:LEU:HB3	1:A:449:LEU:HD13	1.98	0.46
1:C:201:ASN:ND2	1:C:201:ASN:C	2.68	0.46
1:D:32:ASP:O	1:D:38:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:LYS:HB2	1:D:174:VAL:HG23	1.97	0.46
1:C:395:PHE:CE2	1:C:397:TRP:CE3	3.04	0.46
1:B:380:ILE:CD1	1:B:386:VAL:HG21	2.45	0.46
1:D:166:TYR:CE1	1:D:255:VAL:HG21	2.50	0.46
1:D:64:ALA:HB1	1:D:321:LEU:HG	1.98	0.46
1:A:69:VAL:O	1:A:69:VAL:HG23	2.16	0.46
1:E:335:MET:HE3	1:E:337:LEU:HD23	1.97	0.46
1:F:306:TYR:CE2	1:F:329:SER:HB3	2.51	0.46
1:E:310:LEU:HD23	1:E:314:ASP:HB2	1.98	0.46
1:A:51:GLU:OE1	1:A:51:GLU:HA	2.16	0.46
1:C:200:ASN:O	1:C:250:GLY:HA2	2.16	0.46
1:F:205:GLN:HA	1:F:207:TRP:CZ3	2.51	0.46
1:E:46:VAL:HG11	2:E:467:GOL:H31	1.98	0.46
1:B:146:VAL:HG21	1:B:261:VAL:CG1	2.46	0.46
1:B:27:ARG:NH1	1:B:49:ILE:HD12	2.30	0.46
1:B:18:SER:OG	1:B:32:ASP:HB2	2.16	0.46
1:C:410:THR:HG23	1:C:412:ALA:H	1.81	0.45
1:D:358:GLN:HB2	1:D:387:VAL:HG12	1.97	0.45
1:A:139:PHE:CD1	1:A:139:PHE:C	2.89	0.45
1:C:78:ARG:NH2	1:C:287:CYS:CB	2.79	0.45
1:C:435:GLU:O	1:C:439:ARG:HG2	2.16	0.45
1:F:329:SER:HB2	1:F:396:ARG:HD2	1.98	0.45
1:C:146:VAL:HG11	1:C:261:VAL:HG11	1.99	0.45
1:D:55:LEU:HD12	1:D:165:PHE:O	2.15	0.45
1:D:45:PHE:CE2	1:D:176:VAL:HG22	2.52	0.45
1:D:356:HIS:HD2	3:D:473:SO4:O3	1.99	0.45
1:C:281:THR:C	1:C:282:ILE:HD13	2.37	0.45
1:A:282:ILE:HG22	1:A:285:ALA:HB2	1.96	0.45
1:E:410:THR:CG2	1:E:416:SER:HA	2.43	0.45
1:A:261:VAL:O	1:A:261:VAL:HG12	2.16	0.45
1:D:226:GLU:H	1:D:226:GLU:CD	2.18	0.45
1:B:242:LEU:HA	1:C:430:TYR:CD1	2.52	0.45
1:F:236:VAL:O	1:F:236:VAL:HG12	2.17	0.45
1:F:418:LEU:HA	1:F:421:LEU:HD22	1.99	0.45
1:C:236:VAL:O	1:C:240:GLN:HG3	2.16	0.45
1:C:42:GLY:O	1:C:181:LEU:HB2	2.16	0.45
1:B:261:VAL:HG12	1:B:262:ILE:N	2.31	0.45
1:D:231:ALA:HB2	1:E:335:MET:CE	2.47	0.45
1:D:339:GLN:O	1:D:385:SER:HA	2.16	0.45
1:A:348:LEU:HD23	1:A:348:LEU:C	2.37	0.45
1:A:294:PRO:HB3	1:A:300:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:GLN:NE2	1:C:391:THR:HG21	2.24	0.45
1:A:360:VAL:CG1	1:C:222:GLY:HA3	2.46	0.45
1:C:13:ASN:N	1:C:13:ASN:HD22	2.15	0.45
1:D:371:GLN:NE2	1:D:391:THR:HG21	2.32	0.45
1:F:267:ARG:CG	1:F:267:ARG:NH2	2.75	0.45
1:D:358:GLN:NE2	1:F:227:VAL:HG11	2.32	0.45
1:E:350:VAL:HB	1:E:373:SER:O	2.17	0.45
1:F:23:ALA:HB3	1:F:26:GLY:O	2.17	0.45
1:D:189:ASP:C	1:D:191:ASN:H	2.20	0.45
1:C:423:LEU:HA	1:C:423:LEU:HD23	1.73	0.45
1:C:223:PHE:HB2	1:C:228:LEU:HD13	1.98	0.45
1:D:298:ASP:OD2	1:D:309:THR:HB	2.16	0.45
1:C:317:ILE:HD12	1:C:317:ILE:HA	1.85	0.45
1:E:297:ALA:HA	1:E:308:SER:HB2	1.99	0.45
1:A:69:VAL:HG23	1:A:152:GLY:N	2.32	0.44
1:A:211:ARG:CD	1:B:8:GLN:HE22	2.26	0.44
1:A:453:SER:C	1:C:230:LYS:NZ	2.70	0.44
1:D:234:ILE:HD11	1:D:239:ALA:HA	1.99	0.44
1:B:372:VAL:HG13	1:B:372:VAL:O	2.17	0.44
1:A:81:PRO:HB3	1:B:408:ILE:O	2.17	0.44
1:F:62:SER:O	1:F:186:ASN:HA	2.16	0.44
1:B:85:GLU:HG3	1:B:144:GLN:CG	2.48	0.44
1:E:324:SER:CB	1:E:403:ASN:O	2.65	0.44
1:D:215:PRO:O	1:D:217:LYS:NZ	2.50	0.44
1:B:303:GLN:O	1:B:331:ARG:HD3	2.17	0.44
1:F:15:LEU:HD12	1:F:37:GLN:OE1	2.17	0.44
1:D:263:ARG:N	1:D:264:PRO:CD	2.67	0.44
1:F:348:LEU:O	1:F:377:LEU:HA	2.17	0.44
1:E:86:THR:HG22	1:E:142:MET:HG2	1.99	0.44
1:A:87:PHE:HD1	1:A:262:ILE:HG23	1.81	0.44
1:C:419:ARG:O	1:C:441:LYS:HE2	2.17	0.44
1:B:337:LEU:O	1:B:339:GLN:HG2	2.18	0.44
1:B:295:SER:HB2	1:B:296:ASN:OD1	2.17	0.44
1:D:221:ASN:HD22	1:D:243:GLN:HB3	1.83	0.44
1:D:282:ILE:HG22	1:D:285:ALA:N	2.32	0.44
1:F:359:VAL:O	1:F:367:VAL:HG22	2.18	0.44
1:B:63:THR:HG21	1:B:181:LEU:HD12	2.00	0.44
1:D:76:MET:HG3	1:D:76:MET:O	2.11	0.44
1:A:205:GLN:HA	1:A:207:TRP:CZ3	2.52	0.44
1:C:321:LEU:C	1:C:322:ARG:HG2	2.38	0.44
1:E:150:ARG:HG2	1:E:151:THR:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:VAL:HG23	1:C:83:CYS:SG	2.57	0.44
1:D:303:GLN:O	1:D:331:ARG:HD3	2.18	0.44
1:D:43:VAL:HG21	1:D:347:VAL:HG21	2.00	0.44
1:B:262:ILE:CD1	1:B:263:ARG:HH11	2.30	0.44
1:E:346:ALA:HB3	1:E:380:ILE:HB	2.00	0.44
1:D:307:ILE:CG2	1:D:326:LEU:HD21	2.48	0.44
1:F:350:VAL:CG2	1:F:372:VAL:HG13	2.45	0.44
1:A:176:VAL:HG21	1:A:349:TYR:CZ	2.53	0.44
1:E:387:VAL:HG13	1:E:387:VAL:O	2.18	0.44
1:F:12:LEU:O	1:F:13:ASN:ND2	2.51	0.44
1:A:260:SER:HB2	1:A:263:ARG:CD	2.39	0.44
1:E:193:ARG:HH22	1:F:8:GLN:HE21	1.57	0.44
1:B:324:SER:CB	1:B:403:ASN:O	2.64	0.44
1:D:223:PHE:CE1	1:E:387:VAL:HG12	2.53	0.44
1:E:223:PHE:O	1:E:243:GLN:NE2	2.51	0.44
1:C:155:ILE:N	1:C:155:ILE:HD12	2.33	0.44
1:C:291:LEU:HD21	1:C:310:LEU:HG	1.99	0.44
1:B:146:VAL:HG12	1:B:147:GLU:N	2.33	0.44
1:D:342:ALA:HB1	1:F:160:GLY:HA3	1.99	0.44
1:A:380:ILE:HG21	1:A:386:VAL:CG2	2.48	0.44
1:C:288:THR:HG22	1:C:289:ASP:N	2.33	0.44
1:B:304:LEU:HD12	1:B:304:LEU:HA	1.63	0.44
1:D:309:THR:HG23	1:D:310:LEU:N	2.33	0.43
1:A:243:GLN:O	1:A:244:ASN:C	2.56	0.43
1:C:326:LEU:HB3	1:C:399:GLU:HB2	2.00	0.43
1:A:227:VAL:HG21	1:B:387:VAL:HG11	1.99	0.43
1:D:224:THR:HG23	1:E:358:GLN:HE22	1.83	0.43
1:D:42:GLY:O	1:D:181:LEU:HB2	2.18	0.43
1:E:205:GLN:HA	1:E:207:TRP:CZ3	2.52	0.43
1:C:228:LEU:HA	1:C:228:LEU:HD12	1.78	0.43
1:B:423:LEU:HD23	1:B:423:LEU:HA	1.88	0.43
1:B:81:PRO:HG2	1:C:407:GLN:CG	2.48	0.43
1:A:362:ASP:HB3	1:C:195:PHE:CE1	2.53	0.43
1:C:312:SER:O	1:C:316:PRO:HA	2.18	0.43
1:C:446:GLU:H	1:C:446:GLU:HG2	1.46	0.43
1:E:224:THR:O	1:E:227:VAL:HG12	2.18	0.43
1:E:57:LEU:HD11	1:E:253:ILE:HG12	2.00	0.43
1:B:80:VAL:HB	1:B:81:PRO:CD	2.48	0.43
1:F:88:GLN:HG2	1:F:140:ARG:HG3	2.00	0.43
1:E:230:LYS:HZ3	1:F:454:GLY:HA2	1.84	0.43
1:F:33:HIS:CE1	1:F:192:PRO:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:O	1:B:252:ILE:HA	2.18	0.43
1:A:211:ARG:HD2	1:B:8:GLN:NE2	2.31	0.43
1:E:439:ARG:HB2	1:E:443:ASN:CG	2.39	0.43
1:D:158:HIS:CE1	1:D:317:ILE:HD11	2.50	0.43
1:C:346:ALA:HA	1:C:400:PHE:O	2.18	0.43
1:F:434:LEU:HA	1:F:434:LEU:HD12	1.78	0.43
1:A:94:GLN:HB2	1:A:138:GLY:HA3	2.01	0.43
1:B:212:GLU:OE1	1:F:37:GLN:NE2	2.51	0.43
1:B:232:PHE:CE1	1:C:412:ALA:HB2	2.53	0.43
1:A:62:SER:O	1:A:186:ASN:HA	2.19	0.43
1:F:389:ARG:CZ	1:F:454:GLY:HA3	2.49	0.43
1:C:47:ARG:HG3	1:C:176:VAL:HG23	2.01	0.43
1:C:13:ASN:N	1:C:13:ASN:ND2	2.67	0.43
1:A:332:GLN:O	1:A:333:ASN:HB2	2.19	0.43
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.77	0.43
1:A:211:ARG:HE	1:A:211:ARG:CA	2.29	0.43
1:A:63:THR:HG21	1:A:181:LEU:HD12	2.01	0.43
1:E:38:LEU:HA	1:E:38:LEU:HD23	1.78	0.43
1:D:13:ASN:H	1:D:37:GLN:HE22	1.65	0.43
1:B:160:GLY:HA3	1:C:342:ALA:HB1	2.00	0.43
1:A:205:GLN:NE2	1:A:211:ARG:NH1	2.67	0.42
1:C:326:LEU:HD22	1:C:399:GLU:CD	2.39	0.42
1:B:157:THR:OG1	1:B:163:GLN:NE2	2.52	0.42
1:B:234:ILE:HD11	1:B:239:ALA:HA	2.00	0.42
1:C:339:GLN:HB2	1:C:408:ILE:HG22	2.00	0.42
1:F:245:GLN:C	1:F:246:GLN:HG2	2.40	0.42
1:E:303:GLN:O	1:E:331:ARG:HD3	2.19	0.42
1:A:92:VAL:HG23	1:A:93:PHE:N	2.26	0.42
1:A:139:PHE:CE2	1:B:438:ARG:HD2	2.53	0.42
1:A:357:VAL:HG23	1:A:358:GLN:N	2.34	0.42
1:F:157:THR:HG22	1:F:157:THR:O	2.20	0.42
1:E:186:ASN:ND2	1:E:189:ASP:O	2.45	0.42
1:F:211:ARG:HA	1:F:211:ARG:HD2	1.77	0.42
1:E:217:LYS:NZ	1:F:365:ASP:OD1	2.52	0.42
1:F:3:PHE:HD1	1:F:6:GLU:HG2	1.84	0.42
1:A:8:GLN:NE2	1:A:8:GLN:HA	2.34	0.42
1:B:185:GLN:HE22	1:B:321:LEU:HA	1.84	0.42
1:E:61:PHE:HE1	2:E:467:GOL:H32	1.84	0.42
1:B:44:SER:HB2	1:B:192:PRO:HG3	2.02	0.42
1:A:65:LYS:HG3	1:A:179:LEU:HD23	2.00	0.42
1:D:85:GLU:HG3	1:D:144:GLN:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:SER:C	1:F:296:ASN:HD22	2.22	0.42
1:E:345:ASN:O	1:E:401:LYS:HA	2.20	0.42
1:A:5:ASN:ND2	1:C:191:ASN:HD21	2.17	0.42
1:E:317:ILE:HA	1:E:317:ILE:HD12	1.89	0.42
1:F:37:GLN:CG	1:F:379:SER:HB3	2.42	0.42
1:F:286:ARG:HH12	1:F:315:LEU:HD21	1.84	0.42
1:F:69:VAL:HG12	1:F:175:ILE:HG13	2.01	0.42
1:A:77:GLY:O	1:A:163:GLN:HA	2.20	0.42
1:E:283:CYS:O	1:E:283:CYS:SG	2.77	0.42
1:A:73:GLU:HG2	1:A:148:HIS:CE1	2.55	0.42
1:E:280:GLU:N	1:E:320:PHE:CE2	2.88	0.42
1:D:164:TRP:CZ2	1:E:422:PRO:HG2	2.54	0.42
1:F:324:SER:CB	1:F:403:ASN:O	2.68	0.42
1:A:304:LEU:HA	1:A:304:LEU:HD12	1.79	0.42
1:D:17:PRO:HG3	1:D:31:TRP:CH2	2.55	0.42
1:A:339:GLN:HB2	1:A:408:ILE:HG22	2.02	0.42
1:E:225:PRO:HB3	1:E:240:GLN:HG2	2.01	0.42
1:C:326:LEU:O	1:C:326:LEU:HD23	2.19	0.42
1:D:434:LEU:CD2	1:D:434:LEU:H	2.33	0.42
1:A:307:ILE:HG23	1:A:326:LEU:HD21	2.02	0.42
1:E:69:VAL:HG21	1:E:150:ARG:O	2.20	0.42
1:D:217:LYS:HB2	1:D:221:ASN:HB3	2.01	0.42
1:B:245:GLN:C	1:B:247:ASP:H	2.22	0.42
1:A:266:LEU:HD12	1:A:266:LEU:H	1.84	0.42
1:E:380:ILE:HD13	1:E:386:VAL:HG21	2.01	0.42
1:C:397:TRP:CD1	1:C:399:GLU:HG3	2.54	0.42
1:D:71:LYS:HB2	1:D:174:VAL:CG2	2.49	0.42
1:F:371:GLN:NE2	1:F:391:THR:HG21	2.35	0.42
1:B:69:VAL:HG22	1:B:69:VAL:O	2.20	0.41
1:C:71:LYS:HB3	1:C:71:LYS:HE3	1.80	0.41
1:B:231:ALA:CB	1:C:335:MET:HE3	2.48	0.41
1:C:310:LEU:HD13	1:C:318:LEU:HD11	2.00	0.41
1:F:381:PRO:HD2	1:F:384:PHE:CD2	2.55	0.41
1:C:145:LYS:HB3	1:C:145:LYS:HE2	1.81	0.41
1:E:282:ILE:HG22	1:E:285:ALA:N	2.35	0.41
1:E:37:GLN:HG3	1:E:379:SER:HB3	2.02	0.41
1:E:53:LYS:HG2	1:E:166:TYR:OH	2.20	0.41
1:C:225:PRO:HB3	1:C:240:GLN:HG2	2.02	0.41
1:B:303:GLN:HG2	1:B:303:GLN:H	1.64	0.41
1:E:67:SER:OG	1:E:177:SER:HB3	2.20	0.41
1:B:249:ARG:HB3	1:B:253:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:401:LYS:NZ	1:F:408:ILE:HD11	2.36	0.41
1:D:185:GLN:NE2	1:D:321:LEU:HA	2.33	0.41
1:B:64:ALA:HB1	1:B:321:LEU:HG	2.01	0.41
1:E:48:TYR:CZ	1:E:56:TYR:CE1	3.08	0.41
1:E:56:TYR:C	1:E:56:TYR:CD2	2.94	0.41
1:D:436:GLU:HA	1:D:439:ARG:HD2	2.02	0.41
1:E:211:ARG:O	1:E:214:GLN:HG2	2.21	0.41
1:B:329:SER:HB2	1:B:396:ARG:HD2	2.01	0.41
1:A:188:LEU:CD1	1:B:382:GLN:HB3	2.46	0.41
1:A:146:VAL:HG21	1:A:261:VAL:HG11	2.02	0.41
1:D:363:ASN:HA	1:F:216:GLN:HG3	2.03	0.41
1:D:366:ARG:NH2	1:F:224:THR:HG22	2.35	0.41
1:D:446:GLU:HG3	1:D:450:THR:CB	2.50	0.41
1:C:398:ILE:HD13	1:C:399:GLU:N	2.35	0.41
1:D:12:LEU:O	1:D:368:PHE:HD1	2.04	0.41
1:E:361:ASN:C	1:E:361:ASN:OD1	2.59	0.41
1:F:38:LEU:HA	1:F:38:LEU:HD23	1.83	0.41
1:F:348:LEU:C	1:F:348:LEU:HD23	2.41	0.41
1:C:3:PHE:CD1	1:C:4:PRO:HA	2.55	0.41
1:F:301:LYS:HA	1:F:302:PRO:HD3	1.79	0.41
1:B:374:GLN:HG2	1:B:375:GLY:N	2.36	0.41
1:B:77:GLY:HA3	1:B:164:TRP:CZ2	2.55	0.41
1:F:267:ARG:NH2	1:F:267:ARG:HG3	2.36	0.41
1:D:315:LEU:O	1:D:317:ILE:N	2.54	0.41
1:D:387:VAL:HG11	1:F:227:VAL:HG21	2.03	0.41
1:E:350:VAL:HG12	1:E:374:GLN:HA	2.01	0.41
1:F:373:SER:O	1:F:374:GLN:C	2.57	0.41
1:D:324:SER:HB2	1:D:403:ASN:O	2.21	0.41
1:D:327:ARG:HH12	1:D:351:THR:HG21	1.85	0.41
1:D:333:ASN:OD1	1:D:389:ARG:NH1	2.54	0.41
1:D:245:GLN:HE21	1:D:245:GLN:HB3	1.66	0.41
1:B:351:THR:HG22	1:B:352:ASP:CG	2.41	0.41
1:A:205:GLN:HE22	1:A:211:ARG:HH11	1.69	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.78	0.41
1:C:326:LEU:CD2	1:C:326:LEU:C	2.87	0.41
1:B:71:LYS:HB2	1:B:174:VAL:HG23	2.01	0.41
1:C:33:HIS:CE1	1:C:192:PRO:HD2	2.56	0.41
1:D:160:GLY:HA3	1:E:342:ALA:CB	2.41	0.41
1:B:261:VAL:HG22	1:C:422:PRO:HB3	2.02	0.41
1:A:335:MET:HE2	1:A:450:THR:CG2	2.51	0.41
1:A:140:ARG:HD2	1:A:140:ARG:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:PRO:HD2	1:D:226:GLU:OE1	2.21	0.41
1:E:447:THR:HG22	1:E:448:THR:OG1	2.21	0.41
1:F:57:LEU:HD11	1:F:253:ILE:HD13	2.03	0.41
1:A:88:GLN:HB3	1:A:88:GLN:HE21	1.65	0.41
1:D:216:GLN:HG3	1:E:363:ASN:HA	2.03	0.41
1:D:380:ILE:HD13	1:D:386:VAL:HG21	2.03	0.41
1:B:13:ASN:H	1:B:37:GLN:HE22	1.67	0.41
1:C:419:ARG:HH12	1:C:442:PHE:HA	1.86	0.41
1:D:231:ALA:CA	1:E:335:MET:HE2	2.50	0.41
1:A:232:PHE:HB2	1:A:234:ILE:HG12	2.03	0.41
1:D:372:VAL:HG13	1:D:372:VAL:O	2.21	0.41
1:A:78:ARG:HD3	1:A:163:GLN:HE21	1.86	0.41
1:E:298:ASP:OD2	1:E:309:THR:HB	2.21	0.41
1:A:318:LEU:HA	1:A:318:LEU:HD23	1.88	0.41
1:F:66:LEU:HA	1:F:66:LEU:HD23	1.87	0.41
1:B:77:GLY:HA3	1:B:164:TRP:NE1	2.34	0.40
1:D:244:ASN:HA	1:D:244:ASN:HD22	1.73	0.40
1:F:30:VAL:HG21	1:F:207:TRP:HB3	2.04	0.40
1:F:267:ARG:HH21	1:F:267:ARG:HG3	1.86	0.40
1:A:331:ARG:O	1:A:332:GLN:C	2.59	0.40
1:A:363:ASN:ND2	1:A:365:ASP:OD2	2.42	0.40
1:A:330:ILE:HG12	1:A:395:PHE:HB3	2.04	0.40
1:F:71:LYS:HE2	1:F:71:LYS:HB3	1.55	0.40
1:D:310:LEU:HA	1:D:310:LEU:HD23	1.79	0.40
1:A:361:ASN:HD22	1:A:361:ASN:C	2.25	0.40
1:E:228:LEU:HD12	1:E:228:LEU:HA	1.74	0.40
1:A:258:PRO:C	1:A:260:SER:H	2.25	0.40
1:F:437:ALA:HA	1:F:440:VAL:CG1	2.51	0.40
1:A:205:GLN:HE21	1:A:211:ARG:HD3	1.85	0.40
1:B:347:VAL:HG12	1:B:400:PHE:HB2	2.04	0.40
1:F:78:ARG:CD	1:F:163:GLN:HE21	2.34	0.40
1:A:291:LEU:HB3	1:A:327:ARG:HB3	2.02	0.40
1:B:310:LEU:HA	1:B:310:LEU:HD23	1.80	0.40
1:A:434:LEU:HD12	1:A:434:LEU:HA	1.79	0.40
1:A:200:ASN:OD1	1:A:217:LYS:HA	2.21	0.40
1:A:63:THR:HG22	1:A:186:ASN:CB	2.45	0.40
1:C:69:VAL:CG2	1:C:150:ARG:O	2.69	0.40
1:E:76:MET:HG2	1:E:149:ILE:HG21	2.03	0.40
1:A:24:GLU:OE1	1:A:249:ARG:HD2	2.21	0.40
1:A:65:LYS:HB3	1:A:157:THR:HB	2.03	0.40
1:A:421:LEU:CD1	1:C:79:VAL:HG21	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:ASP:HA	1:F:294:PRO:HD3	1.72	0.40
1:B:78:ARG:CZ	1:B:287:CYS:HB2	2.52	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	392/466 (84%)	353 (90%)	33 (8%)	6 (2%)	13	48
1	B	381/466 (82%)	350 (92%)	29 (8%)	2 (0%)	34	75
1	C	381/466 (82%)	350 (92%)	25 (7%)	6 (2%)	12	46
1	D	384/466 (82%)	354 (92%)	28 (7%)	2 (0%)	34	75
1	E	383/466 (82%)	339 (88%)	39 (10%)	5 (1%)	15	52
1	F	391/466 (84%)	349 (89%)	36 (9%)	6 (2%)	13	48
All	All	2312/2796 (83%)	2095 (91%)	190 (8%)	27 (1%)	16	54

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	PRO
1	C	333	ASN
1	A	92	VAL
1	A	244	ASN
1	B	6	GLU
1	D	264	PRO
1	E	263	ARG
1	F	82	GLY
1	F	264	PRO
1	A	264	PRO

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Mol	Chain	Res	Type
1	C	81	PRO
1	C	263	ARG
1	E	333	ASN
1	F	6	GLU
1	A	263	ARG
1	C	332	GLN
1	D	210	GLY
1	E	3	PHE
1	E	81	PRO
1	F	71	LYS
1	A	416	SER
1	B	258	PRO
1	C	285	ALA
1	F	265	PRO
1	C	3	PHE
1	E	262	ILE
1	F	263	ARG

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	343/388 (88%)	298 (87%)	45 (13%)	5 20
1	B	333/388 (86%)	277 (83%)	56 (17%)	2 12
1	C	333/388 (86%)	294 (88%)	39 (12%)	7 25
1	D	335/388 (86%)	293 (88%)	42 (12%)	6 22
1	E	334/388 (86%)	291 (87%)	43 (13%)	5 21
1	F	342/388 (88%)	297 (87%)	45 (13%)	5 20
All	All	2020/2328 (87%)	1750 (87%)	270 (13%)	5 19

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO

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Mol	Chain	Res	Type
1	A	6	GLU
1	A	30	VAL
1	A	52	SER
1	A	66	LEU
1	A	71	LYS
1	A	86	THR
1	A	88	GLN
1	A	94	GLN
1	A	140	ARG
1	A	144	GLN
1	A	157	THR
1	A	158	HIS
1	A	171	GLN
1	A	181	LEU
1	A	187	GLN
1	A	189	ASP
1	A	191	ASN
1	A	211	ARG
1	A	217	LYS
1	A	220	LEU
1	A	226	GLU
1	A	245	GLN
1	A	252	ILE
1	A	256	GLN
1	A	260	SER
1	A	266	LEU
1	A	282	ILE
1	A	303	GLN
1	A	304	LEU
1	A	308	SER
1	A	314	ASP
1	A	317	ILE
1	A	329	SER
1	A	357	VAL
1	A	361	ASN
1	A	385	SER
1	A	388	LYS
1	A	391	THR
1	A	398	ILE
1	A	421	LEU
1	A	423	LEU
1	A	434	LEU

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Mol	Chain	Res	Type
1	A	438	ARG
1	A	446	GLU
1	B	6	GLU
1	B	9	LEU
1	B	11	GLN
1	B	27	ARG
1	B	30	VAL
1	B	37	GLN
1	B	66	LEU
1	B	69	VAL
1	B	76	MET
1	B	142	MET
1	B	145	LYS
1	B	150	ARG
1	B	168	ASP
1	B	176	VAL
1	B	179	LEU
1	B	181	LEU
1	B	188	LEU
1	B	190	ARG
1	B	191	ASN
1	B	197	LEU
1	B	211	ARG
1	B	214	GLN
1	B	217	LYS
1	B	220	LEU
1	B	228	LEU
1	B	235	ASP
1	B	237	ARG
1	B	238	THR
1	B	248	ASN
1	B	258	PRO
1	B	262	ILE
1	B	263	ARG
1	B	267	ARG
1	B	282	ILE
1	B	296	ASN
1	B	299	VAL
1	B	304	LEU
1	B	308	SER
1	B	309	THR
1	B	310	LEU

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Mol	Chain	Res	Type
1	B	322	ARG
1	B	332	GLN
1	B	339	GLN
1	B	357	VAL
1	B	361	ASN
1	B	385	SER
1	B	388	LYS
1	B	398	ILE
1	B	409	ASN
1	B	421	LEU
1	B	433	SER
1	B	434	LEU
1	B	438	ARG
1	B	440	VAL
1	B	445	ILE
1	B	447	THR
1	C	5	ASN
1	C	6	GLU
1	C	9	LEU
1	C	13	ASN
1	C	30	VAL
1	C	37	GLN
1	C	50	ILE
1	C	66	LEU
1	C	71	LYS
1	C	76	MET
1	C	158	HIS
1	C	176	VAL
1	C	177	SER
1	C	181	LEU
1	C	189	ASP
1	C	190	ARG
1	C	197	LEU
1	C	211	ARG
1	C	217	LYS
1	C	220	LEU
1	C	235	ASP
1	C	256	GLN
1	C	303	GLN
1	C	304	LEU
1	C	310	LEU
1	C	322	ARG

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Mol	Chain	Res	Type
1	C	324	SER
1	C	347	VAL
1	C	351	THR
1	C	357	VAL
1	C	361	ASN
1	C	386	VAL
1	C	393	GLU
1	C	398	ILE
1	C	410	THR
1	C	421	LEU
1	C	434	LEU
1	C	439	ARG
1	C	446	GLU
1	D	2	GLN
1	D	6	GLU
1	D	9	LEU
1	D	27	ARG
1	D	30	VAL
1	D	53	LYS
1	D	76	MET
1	D	80	VAL
1	D	140	ARG
1	D	145	LYS
1	D	150	ARG
1	D	158	HIS
1	D	168	ASP
1	D	171	GLN
1	D	179	LEU
1	D	181	LEU
1	D	187	GLN
1	D	188	LEU
1	D	189	ASP
1	D	197	LEU
1	D	211	ARG
1	D	217	LYS
1	D	219	ILE
1	D	220	LEU
1	D	226	GLU
1	D	237	ARG
1	D	260	SER
1	D	263	ARG
1	D	299	VAL

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Mol	Chain	Res	Type
1	D	301	LYS
1	D	303	GLN
1	D	304	LEU
1	D	308	SER
1	D	309	THR
1	D	354	GLU
1	D	361	ASN
1	D	372	VAL
1	D	374	GLN
1	D	398	ILE
1	D	421	LEU
1	D	438	ARG
1	D	446	GLU
1	E	9	LEU
1	E	30	VAL
1	E	37	GLN
1	E	66	LEU
1	E	69	VAL
1	E	76	MET
1	E	140	ARG
1	E	148	HIS
1	E	150	ARG
1	E	177	SER
1	E	181	LEU
1	E	189	ASP
1	E	190	ARG
1	E	195	PHE
1	E	211	ARG
1	E	214	GLN
1	E	217	LYS
1	E	220	LEU
1	E	226	GLU
1	E	228	LEU
1	E	235	ASP
1	E	260	SER
1	E	295	SER
1	E	303	GLN
1	E	304	LEU
1	E	308	SER
1	E	310	LEU
1	E	329	SER
1	E	331	ARG

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Mol	Chain	Res	Type
1	E	335	MET
1	E	341	ASN
1	E	347	VAL
1	E	354	GLU
1	E	357	VAL
1	E	372	VAL
1	E	386	VAL
1	E	388	LYS
1	E	391	THR
1	E	410	THR
1	E	418	LEU
1	E	439	ARG
1	E	445	ILE
1	E	446	GLU
1	F	6	GLU
1	F	30	VAL
1	F	37	GLN
1	F	41	SER
1	F	66	LEU
1	F	76	MET
1	F	83	CYS
1	F	85	GLU
1	F	88	GLN
1	F	90	SER
1	F	140	ARG
1	F	145	LYS
1	F	157	THR
1	F	158	HIS
1	F	176	VAL
1	F	177	SER
1	F	197	LEU
1	F	217	LYS
1	F	220	LEU
1	F	226	GLU
1	F	248	ASN
1	F	260	SER
1	F	267	ARG
1	F	284	SER
1	F	286	ARG
1	F	288	THR
1	F	289	ASP
1	F	296	ASN

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Mol	Chain	Res	Type
1	F	303	GLN
1	F	304	LEU
1	F	310	LEU
1	F	317	ILE
1	F	347	VAL
1	F	357	VAL
1	F	372	VAL
1	F	385	SER
1	F	391	THR
1	F	410	THR
1	F	421	LEU
1	F	434	LEU
1	F	435	GLU
1	F	438	ARG
1	F	440	VAL
1	F	447	THR
1	F	449	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	2	GLN
1	A	5	ASN
1	A	37	GLN
1	A	88	GLN
1	A	144	GLN
1	A	163	GLN
1	A	167	ASN
1	A	171	GLN
1	A	184	HIS
1	A	205	GLN
1	A	214	GLN
1	A	245	GLN
1	A	251	ASN
1	A	256	GLN
1	A	303	GLN
1	A	311	ASN
1	A	339	GLN
1	A	361	ASN
1	A	371	GLN
1	A	407	GLN

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Mol	Chain	Res	Type
1	B	11	GLN
1	B	143	HIS
1	B	158	HIS
1	B	163	GLN
1	B	167	ASN
1	B	184	HIS
1	B	185	GLN
1	B	203	GLN
1	B	244	ASN
1	B	245	GLN
1	B	251	ASN
1	B	303	GLN
1	B	311	ASN
1	B	339	GLN
1	B	361	ASN
1	B	443	ASN
1	C	5	ASN
1	C	163	GLN
1	C	167	ASN
1	C	185	GLN
1	C	201	ASN
1	C	214	GLN
1	C	244	ASN
1	C	251	ASN
1	C	256	GLN
1	C	296	ASN
1	C	311	ASN
1	C	339	GLN
1	C	341	ASN
1	C	371	GLN
1	C	409	ASN
1	C	443	ASN
1	C	451	HIS
1	D	2	GLN
1	D	13	ASN
1	D	37	GLN
1	D	148	HIS
1	D	158	HIS
1	D	185	GLN
1	D	187	GLN
1	D	214	GLN
1	D	244	ASN

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Mol	Chain	Res	Type
1	D	245	GLN
1	D	248	ASN
1	D	251	ASN
1	D	303	GLN
1	D	311	ASN
1	D	339	GLN
1	D	356	HIS
1	D	361	ASN
1	D	371	GLN
1	D	443	ASN
1	E	1	GLN
1	E	2	GLN
1	E	37	GLN
1	E	167	ASN
1	E	184	HIS
1	E	187	GLN
1	E	200	ASN
1	E	203	GLN
1	E	240	GLN
1	E	256	GLN
1	E	339	GLN
1	E	371	GLN
1	E	409	ASN
1	E	443	ASN
1	F	8	GLN
1	F	11	GLN
1	F	13	ASN
1	F	37	GLN
1	F	88	GLN
1	F	163	GLN
1	F	167	ASN
1	F	248	ASN
1	F	256	GLN
1	F	296	ASN
1	F	311	ASN
1	F	371	GLN
1	F	405	ASN
1	F	407	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)

10 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	$\#\|Z\| > 2$
2	GOL	A	467	-	5,5,5	0.27	0	5,5,5	0.69	0
3	SO4	A	474	-	4,4,4	0.19	0	6,6,6	0.08	0
2	GOL	B	467	-	5,5,5	0.39	0	5,5,5	0.83	0
2	GOL	C	467	-	5,5,5	0.35	0	5,5,5	0.82	0
3	SO4	C	472	-	4,4,4	0.13	0	6,6,6	0.25	0
2	GOL	D	467	-	5,5,5	0.30	0	5,5,5	1.11	0
3	SO4	D	473	-	4,4,4	0.11	0	6,6,6	0.24	0
2	GOL	E	467	-	5,5,5	0.28	0	5,5,5	0.90	0
2	GOL	F	467	-	5,5,5	0.38	0	5,5,5	0.40	0
3	SO4	F	475	-	4,4,4	0.16	0	6,6,6	0.16	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
2	GOL	A	467	-	-	0/4/4/4	0/0/0/0
3	SO4	A	474	-	-	0/0/0/0	0/0/0/0
2	GOL	B	467	-	-	0/4/4/4	0/0/0/0
2	GOL	C	467	-	-	0/4/4/4	0/0/0/0
3	SO4	C	472	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	467	-	-	0/4/4/4	0/0/0/0
3	SO4	D	473	-	-	0/0/0/0	0/0/0/0
2	GOL	E	467	-	-	0/4/4/4	0/0/0/0
2	GOL	F	467	-	-	0/4/4/4	0/0/0/0
3	SO4	F	475	-	-	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.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	467	GOL	1	0
3	A	474	SO4	1	0
2	B	467	GOL	1	0
2	C	467	GOL	1	0
2	D	467	GOL	4	0
3	D	473	SO4	1	0
2	E	467	GOL	4	0
2	F	467	GOL	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	A	398/466 (85%)	0.25	20 (5%)	32	17	22, 44, 114, 161	0
1	B	387/466 (83%)	0.15	9 (2%)	64	41	18, 41, 99, 161	0
1	C	387/466 (83%)	0.15	5 (1%)	79	59	20, 44, 101, 130	0
1	D	390/466 (83%)	0.15	7 (1%)	71	49	20, 42, 105, 143	0
1	E	389/466 (83%)	0.15	10 (2%)	59	37	22, 45, 99, 154	0
1	F	396/466 (84%)	0.25	18 (4%)	37	20	20, 45, 111, 160	0
All	All	2347/2796 (83%)	0.18	69 (2%)	55	33	18, 43, 105, 161	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	455	PRO	7.1
1	A	86	THR	6.1
1	F	87	PHE	5.3
1	A	87	PHE	5.2
1	E	138	GLY	5.1
1	B	264	PRO	5.0
1	A	138	GLY	5.0
1	F	262	ILE	4.9
1	E	139	PHE	4.4
1	A	94	GLN	4.2
1	F	138	GLY	4.2
1	A	90	SER	4.1
1	A	89	ASP	4.1
1	F	91	SER	4.1
1	A	2	GLN	4.0
1	A	95	PRO	4.0
1	A	93	PHE	4.0
1	E	86	THR	3.7
1	F	259	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	84	ALA	3.5
1	C	86	THR	3.3
1	A	262	ILE	3.2
1	E	261	VAL	3.2
1	B	82	GLY	3.1
1	F	268	SER	3.1
1	C	286	ARG	3.0
1	F	88	GLN	3.0
1	D	453	SER	3.0
1	D	455	PRO	3.0
1	C	261	VAL	2.9
1	A	88	GLN	2.9
1	F	267	ARG	2.7
1	B	453	SER	2.7
1	F	264	PRO	2.7
1	E	2	GLN	2.6
1	B	81	PRO	2.6
1	F	81	PRO	2.6
1	D	286	ARG	2.6
1	B	455	PRO	2.5
1	D	3	PHE	2.5
1	F	85	GLU	2.5
1	A	92	VAL	2.5
1	F	86	THR	2.5
1	F	90	SER	2.5
1	B	3	PHE	2.4
1	B	281	THR	2.4
1	E	455	PRO	2.4
1	E	85	GLU	2.4
1	A	84	ALA	2.4
1	C	2	GLN	2.4
1	F	89	ASP	2.4
1	A	265	PRO	2.3
1	F	139	PHE	2.3
1	A	259	PHE	2.2
1	A	140	ARG	2.2
1	A	91	SER	2.2
1	E	82	GLY	2.2
1	A	81	PRO	2.1
1	E	264	PRO	2.1
1	A	1	GLN	2.1
1	E	262	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	2	GLN	2.1
1	D	262	ILE	2.1
1	F	92	VAL	2.1
1	F	142	MET	2.0
1	A	434	LEU	2.0
1	C	84	ALA	2.0
1	D	82	GLY	2.0
1	B	260	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	A	474	5/5	0.95	0.56	9.14	54,129,166,174	0
3	SO4	D	473	5/5	0.88	0.31	3.52	49,84,97,194	0
2	GOL	A	467	6/6	0.98	0.25	1.29	16,20,31,52	0
3	SO4	F	475	5/5	0.96	0.35	0.53	66,92,136,148	0
2	GOL	E	467	6/6	0.94	0.21	0.44	18,28,35,40	0
2	GOL	C	467	6/6	0.97	0.21	0.13	17,32,33,41	0
2	GOL	D	467	6/6	0.97	0.19	-0.18	23,28,34,72	0
3	SO4	C	472	5/5	0.85	0.17	-0.52	59,87,126,187	0
2	GOL	B	467	6/6	0.98	0.19	-0.68	16,29,38,49	0
2	GOL	F	467	6/6	0.98	0.19	-0.89	11,28,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.