Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:54 AM GMT

PDB ID	:	3CLQ
Title	:	Crystal structure of a conserved protein of unknown function from Enterococcus faecalis V583
Authors	:	Tan, K.; Duggan, E.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-03-19
Resolution	:	2.50 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:

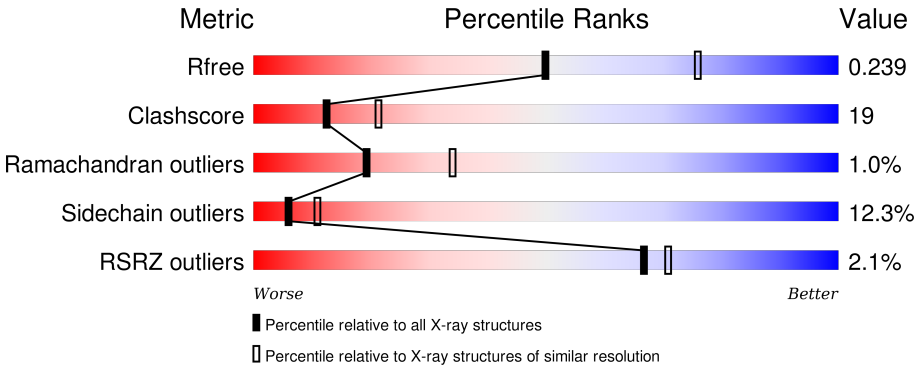
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	421	71% 23% 6%
1	B	421	64% 28% 7%
1	C	421	63% 30% 7%
1	D	421	66% 27% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	C	4	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12653 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.

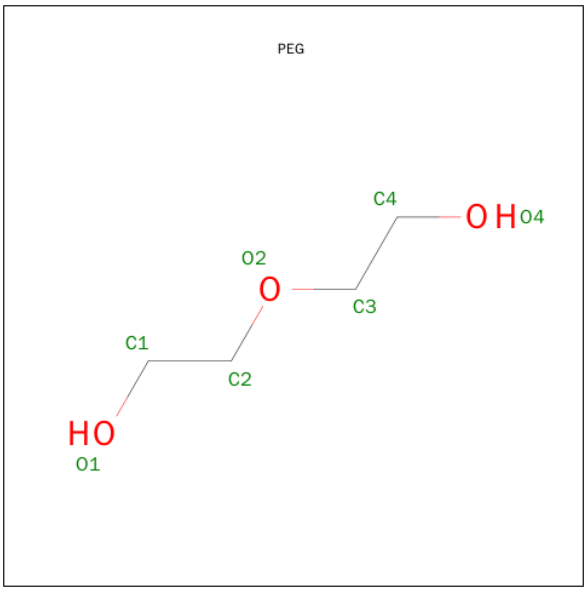
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	Se	0	0	0
			3143	1985	528	604	6	20			
1	B	421	Total	C	N	O	S	Se	0	0	0
			3149	1988	529	606	6	20			
1	C	421	Total	C	N	O	S	Se	0	0	0
			3149	1988	529	606	6	20			
1	D	419	Total	C	N	O	S	Se	0	0	0
			3135	1981	526	602	6	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	SER	-	EXPRESSION TAG	UNP Q82ZN9
A	55	ASN	-	EXPRESSION TAG	UNP Q82ZN9
A	56	ALA	-	EXPRESSION TAG	UNP Q82ZN9
B	54	SER	-	EXPRESSION TAG	UNP Q82ZN9
B	55	ASN	-	EXPRESSION TAG	UNP Q82ZN9
B	56	ALA	-	EXPRESSION TAG	UNP Q82ZN9
C	54	SER	-	EXPRESSION TAG	UNP Q82ZN9
C	55	ASN	-	EXPRESSION TAG	UNP Q82ZN9
C	56	ALA	-	EXPRESSION TAG	UNP Q82ZN9
D	54	SER	-	EXPRESSION TAG	UNP Q82ZN9
D	55	ASN	-	EXPRESSION TAG	UNP Q82ZN9
D	56	ALA	-	EXPRESSION TAG	UNP Q82ZN9

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0

- Molecule 3 is water.

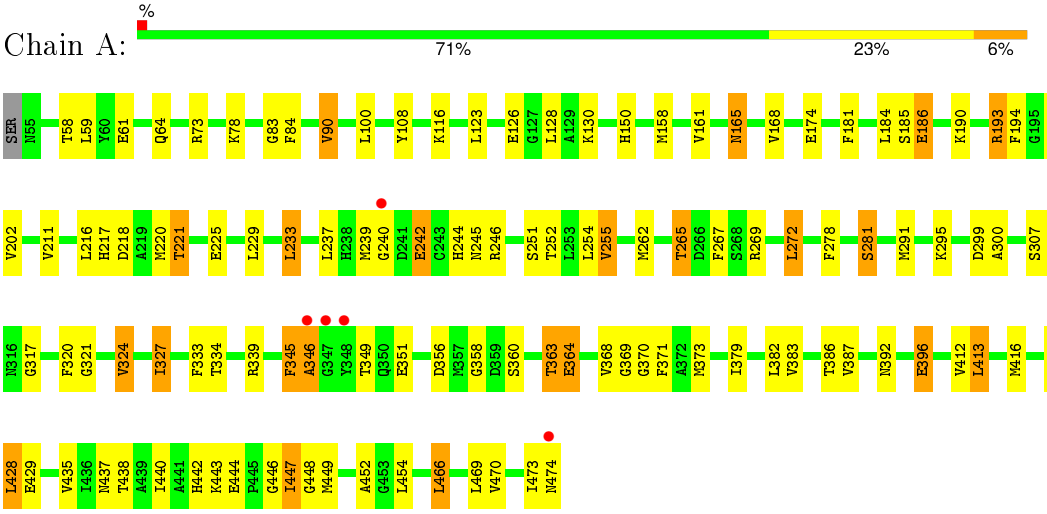
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	B	9	Total O 9 9	0	0
3	C	18	Total O 18 18	0	0
3	D	3	Total O 3 3	0	0

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.

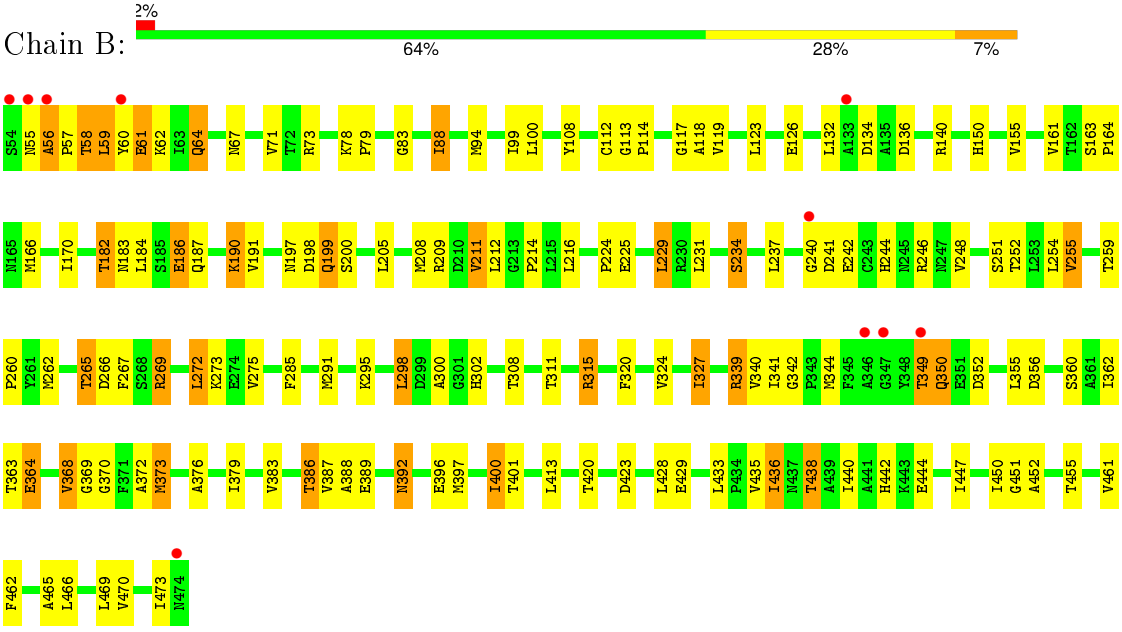
- Molecule 1: Uncharacterized protein

Chain A:



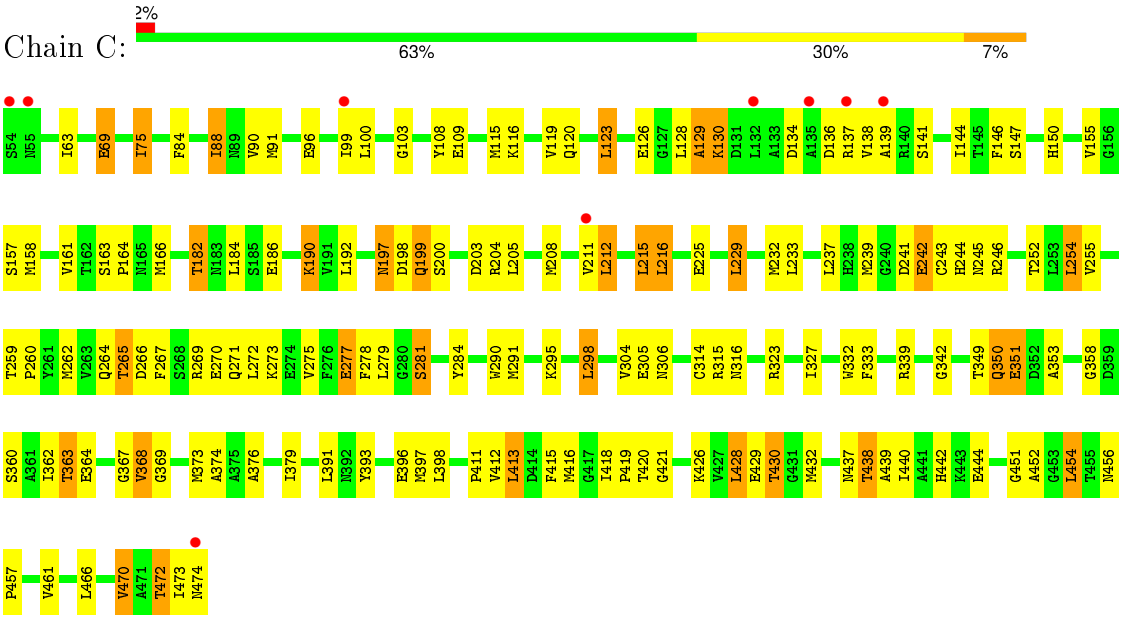
- Molecule 1: Uncharacterized protein

Chain B:



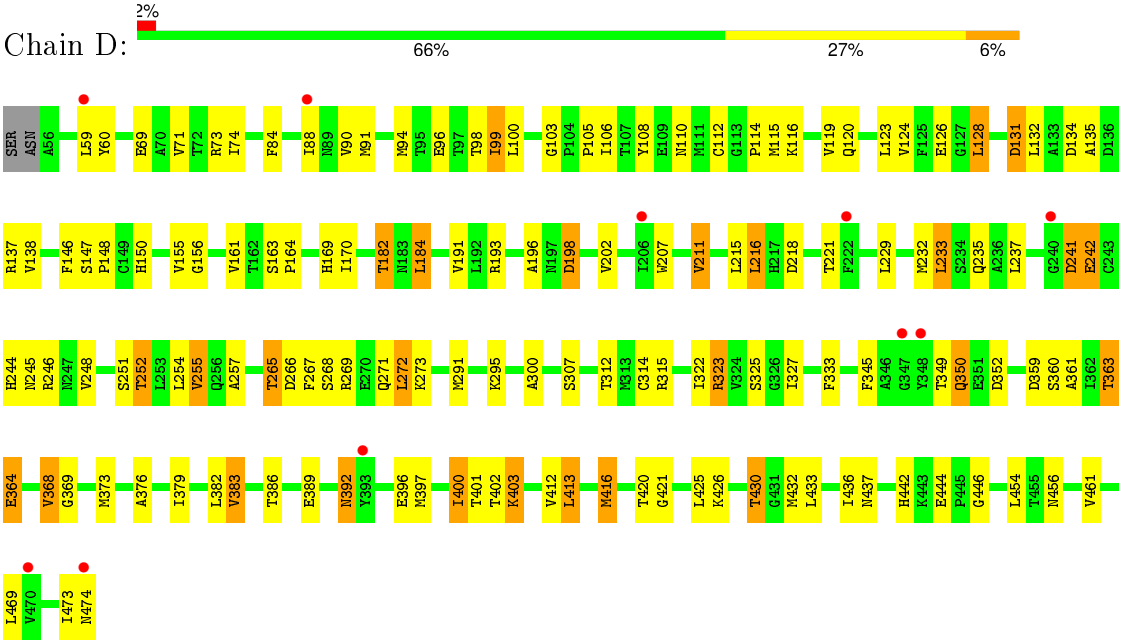
- Molecule 1: Uncharacterized protein

Chain C:



• Molecule 1: Uncharacterized protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.16Å 61.61Å 164.54Å 90.00° 103.94° 90.00°	Depositor
Resolution (Å)	43.03 – 2.50 43.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.7 (43.03-2.50) 88.7 (43.02-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.240 0.184 , 0.239	Depositor DCC
R_{free} test set	3161 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 62658 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12653	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: PEG

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	0.69	0/3186	0.80	2/4300 (0.0%)
1	B	0.58	0/3192	0.71	1/4308 (0.0%)
1	C	0.65	0/3192	0.74	0/4308
1	D	0.59	2/3178 (0.1%)	0.70	2/4289 (0.0%)
All	All	0.63	2/12748 (0.0%)	0.74	5/17205 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	131	ASP	C-O	5.79	1.34	1.23
1	D	128	LEU	CG-CD1	5.29	1.71	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	GLU	C-N-CA	-5.93	106.87	121.70
1	D	233	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	466	LEU	CA-CB-CG	5.27	127.41	115.30
1	D	272	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	186	GLU	N-CA-C	-5.15	97.10	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3143	0	3112	108	0
1	B	3149	0	3117	124	0
1	C	3149	0	3117	140	0
1	D	3135	0	3106	124	0
2	B	14	0	20	3	0
2	C	7	0	10	0	0
2	D	7	0	10	1	0
3	A	19	0	0	0	0
3	B	9	0	0	0	0
3	C	18	0	0	0	0
3	D	3	0	0	0	0
All	All	12653	0	12492	489	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 19.

All (489) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:VAL:O	1:B:182:THR:HG22	1.51	1.09
1:A:447:ILE:HG22	1:A:448:GLY:H	1.16	1.05
1:B:386:THR:HG22	1:B:389:GLU:H	1.23	1.02
1:B:224:PRO:HD2	1:B:225:GLU:OE1	1.60	0.99
1:D:400:ILE:HD11	1:D:430:THR:HG21	1.45	0.98
1:B:340:VAL:HB	1:B:440:ILE:HG22	1.49	0.95
1:A:196:ALA:HA	1:A:446:GLY:HA2	1.46	0.95
1:C:186:GLU:HG2	1:C:208:MSE:HE1	1.46	0.94
1:C:442:HIS:CD2	1:C:444:GLU:HB2	2.02	0.94
1:C:360:SER:O	1:C:363:THR:HB	1.69	0.92
1:B:386:THR:CG2	1:B:389:GLU:H	1.82	0.92
1:D:244:HIS:HB2	1:D:363:THR:HG21	1.51	0.92
1:D:116:LYS:O	1:D:119:VAL:HG22	1.70	0.90
1:A:265:THR:HG22	1:A:267:PHE:H	1.34	0.90
1:C:373:MSE:HE1	1:C:393:TYR:CD2	2.06	0.90
1:D:120:GLN:O	1:D:124:VAL:HG23	1.72	0.89
1:B:265:THR:HG23	1:B:267:PHE:H	1.35	0.89
1:D:426:LYS:O	1:D:430:THR:HB	1.73	0.88
1:D:350:GLN:HE21	1:D:350:GLN:HA	1.36	0.88
1:C:373:MSE:HE1	1:C:393:TYR:HD2	1.37	0.88
1:D:368:VAL:HG13	1:D:369:GLY:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LYS:O	1:C:120:GLN:HG3	1.75	0.85
1:A:447:ILE:HG22	1:A:448:GLY:N	1.91	0.85
1:C:368:VAL:HG13	1:C:369:GLY:H	1.40	0.85
1:B:442:HIS:HD2	1:B:444:GLU:H	1.21	0.84
1:C:442:HIS:HD2	1:C:444:GLU:HB2	1.43	0.84
1:B:324:VAL:O	1:B:327:ILE:HG22	1.77	0.84
1:A:265:THR:CG2	1:A:267:PHE:H	1.90	0.83
1:C:412:VAL:HG13	1:C:413:LEU:HD13	1.59	0.83
1:D:430:THR:HG23	1:D:432:MSE:H	1.43	0.83
1:B:155:VAL:HG23	1:B:182:THR:CG2	2.08	0.83
1:B:73:ARG:HD3	1:B:300:ALA:O	1.79	0.81
1:D:218:ASP:O	1:D:221:THR:HB	1.79	0.81
1:D:430:THR:CG2	1:D:432:MSE:HB2	2.11	0.80
1:B:291:MSE:HE2	1:B:360:SER:HB3	1.61	0.80
1:D:135:ALA:HA	1:D:138:VAL:HG22	1.63	0.79
1:A:245:ASN:HD21	1:A:438:THR:HA	1.47	0.78
1:C:397:MSE:HE1	1:C:432:MSE:HE3	1.66	0.78
1:C:134:ASP:O	1:C:138:VAL:HG13	1.84	0.78
1:C:339:ARG:HH22	1:C:353:ALA:HB3	1.47	0.77
1:A:262:MSE:O	1:A:265:THR:HB	1.83	0.77
1:D:126:GLU:HA	1:D:126:GLU:OE1	1.85	0.77
1:D:400:ILE:CD1	1:D:430:THR:HG21	2.13	0.77
1:A:392:ASN:O	1:A:396:GLU:HG2	1.84	0.76
1:C:204:ARG:HG2	1:C:208:MSE:HE2	1.68	0.75
1:A:58:THR:CG2	1:A:61:GLU:HB2	2.17	0.75
1:C:265:THR:HG23	1:C:267:PHE:H	1.50	0.75
1:A:308:THR:HG22	1:A:469:LEU:HD13	1.67	0.75
1:A:447:ILE:CG2	1:A:448:GLY:H	1.99	0.74
1:D:105:PRO:O	1:D:106:ILE:HG23	1.87	0.74
1:B:155:VAL:O	1:B:182:THR:CG2	2.32	0.74
1:C:200:SER:O	1:C:203:ASP:HB2	1.86	0.74
1:B:269:ARG:HD3	2:B:2:PEG:H32	1.70	0.74
1:C:252:THR:HG22	1:D:252:THR:HB	1.70	0.73
1:C:155:VAL:HG23	1:C:182:THR:HG23	1.70	0.73
1:B:291:MSE:HE2	1:B:360:SER:CB	2.18	0.72
1:D:442:HIS:HD2	1:D:444:GLU:H	1.37	0.72
1:D:134:ASP:O	1:D:138:VAL:HG13	1.88	0.72
1:C:430:THR:CG2	1:C:432:MSE:H	2.03	0.71
1:B:291:MSE:CE	1:B:360:SER:HB3	2.20	0.71
1:B:136:ASP:OD1	1:B:140:ARG:NH1	2.24	0.71
1:A:58:THR:HG23	1:A:61:GLU:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:THR:HG22	1:B:469:LEU:HD13	1.73	0.71
1:A:278:PHE:O	1:A:281:SER:HB2	1.91	0.71
1:C:91:MSE:HE1	1:C:100:LEU:HD11	1.73	0.70
1:C:155:VAL:HG23	1:C:182:THR:CG2	2.22	0.70
1:D:430:THR:HG21	1:D:432:MSE:HB2	1.72	0.70
1:D:368:VAL:CG1	1:D:369:GLY:H	2.04	0.70
1:B:386:THR:HG22	1:B:389:GLU:N	2.01	0.70
1:C:426:LYS:O	1:C:430:THR:HB	1.91	0.70
1:D:397:MSE:CE	1:D:432:MSE:HE1	2.22	0.70
1:C:368:VAL:HG13	1:C:369:GLY:N	2.07	0.70
1:A:252:THR:OG1	1:B:252:THR:HG22	1.92	0.69
1:A:242:GLU:O	1:A:368:VAL:HG13	1.92	0.69
1:D:73:ARG:HD3	1:D:300:ALA:O	1.93	0.69
1:A:364:GLU:OE1	1:A:370:GLY:N	2.26	0.68
1:A:265:THR:CG2	1:A:267:PHE:HD2	2.07	0.68
1:D:265:THR:HG23	1:D:267:PHE:H	1.59	0.68
1:D:430:THR:CG2	1:D:432:MSE:H	2.05	0.68
1:A:368:VAL:HG13	1:A:369:GLY:H	1.56	0.68
1:D:400:ILE:HD11	1:D:430:THR:CG2	2.22	0.68
1:C:245:ASN:ND2	1:C:437:ASN:OD1	2.26	0.68
1:A:442:HIS:HD2	1:A:444:GLU:H	1.40	0.68
1:B:442:HIS:CD2	1:B:444:GLU:HB2	2.30	0.67
1:B:315:ARG:NH1	1:B:436:ILE:HD11	2.10	0.67
1:A:233:LEU:HD12	1:A:233:LEU:C	2.14	0.67
1:C:368:VAL:CG1	1:C:369:GLY:N	2.57	0.67
1:D:155:VAL:O	1:D:182:THR:HG23	1.93	0.67
1:C:123:LEU:HD11	1:C:144:ILE:CD1	2.26	0.66
1:D:150:HIS:HD2	1:D:295:LYS:NZ	1.93	0.66
1:C:430:THR:HG23	1:C:432:MSE:H	1.60	0.66
1:C:265:THR:HG23	1:C:266:ASP:N	2.10	0.66
1:D:84:PHE:CD2	1:D:216:LEU:HB3	2.30	0.66
1:A:373:MSE:HG2	1:A:379:ILE:HD11	1.76	0.66
1:D:291:MSE:HE2	1:D:360:SER:HB2	1.77	0.66
1:A:291:MSE:HE2	1:A:360:SER:HB3	1.78	0.66
1:B:155:VAL:HG23	1:B:182:THR:HG23	1.77	0.65
1:B:100:LEU:O	1:B:161:VAL:HA	1.96	0.65
1:D:350:GLN:CA	1:D:350:GLN:HE21	2.06	0.65
1:A:73:ARG:HD3	1:A:300:ALA:O	1.97	0.65
1:C:456:ASN:HB3	1:C:457:PRO:HD2	1.78	0.65
1:D:368:VAL:CG1	1:D:369:GLY:N	2.60	0.64
1:D:251:SER:O	1:D:255:VAL:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ARG:HH11	1:B:436:ILE:HD11	1.63	0.64
1:C:212:LEU:HD22	1:C:216:LEU:HD22	1.79	0.63
1:C:351:GLU:HG2	1:C:351:GLU:O	1.96	0.63
1:C:430:THR:CG2	1:C:432:MSE:HB2	2.28	0.63
1:B:440:ILE:HG12	1:B:451:GLY:C	2.18	0.63
1:A:190:LYS:NZ	1:A:198:ASP:OD1	2.32	0.63
1:C:373:MSE:HE3	1:C:393:TYR:HB2	1.80	0.63
1:D:265:THR:HG23	1:D:266:ASP:N	2.14	0.62
1:D:312:THR:OG1	1:D:323:ARG:NH1	2.32	0.62
1:D:469:LEU:O	1:D:473:ILE:HG12	1.99	0.62
1:D:312:THR:HB	1:D:323:ARG:HB2	1.81	0.62
1:B:344:MSE:SE	1:B:440:ILE:HD11	2.48	0.62
1:D:442:HIS:CD2	1:D:444:GLU:H	2.17	0.62
1:C:123:LEU:HD11	1:C:144:ILE:HD13	1.82	0.62
1:B:244:HIS:ND1	1:B:364:GLU:OE2	2.31	0.62
1:B:466:LEU:O	1:B:470:VAL:HG13	2.00	0.61
1:B:251:SER:O	1:B:255:VAL:HG13	2.00	0.61
1:C:150:HIS:HD2	1:C:295:LYS:NZ	1.98	0.61
1:A:158:MSE:HB2	1:A:193:ARG:HG3	1.81	0.61
1:C:163:SER:HB2	1:C:164:PRO:CD	2.30	0.61
1:C:376:ALA:O	1:C:379:ILE:HG12	2.00	0.61
1:D:232:MSE:HA	1:D:235:GLN:HE21	1.66	0.61
1:A:473:ILE:O	1:A:474:ASN:HB2	2.02	0.60
1:C:244:HIS:HB2	1:C:363:THR:HG21	1.82	0.60
1:A:265:THR:HG23	1:A:267:PHE:HD2	1.67	0.60
1:D:90:VAL:HG21	1:D:170:ILE:HD13	1.84	0.60
1:C:252:THR:CG2	1:D:252:THR:HB	2.30	0.60
1:A:233:LEU:HD12	1:A:233:LEU:O	2.01	0.60
1:A:185:SER:OG	1:A:186:GLU:O	2.16	0.60
1:B:442:HIS:CD2	1:B:444:GLU:H	2.11	0.60
1:B:155:VAL:HG23	1:B:182:THR:HG21	1.83	0.60
1:C:204:ARG:HG2	1:C:208:MSE:CE	2.31	0.60
1:C:397:MSE:CE	1:C:432:MSE:CE	2.80	0.60
1:D:265:THR:HG23	1:D:267:PHE:HD2	1.66	0.60
1:A:150:HIS:HD2	1:A:295:LYS:NZ	1.99	0.59
1:B:126:GLU:OE2	1:B:163:SER:OG	2.17	0.59
1:B:376:ALA:O	1:B:379:ILE:HG12	2.02	0.59
1:B:108:TYR:CE1	1:B:119:VAL:HG21	2.36	0.59
1:C:278:PHE:O	1:C:281:SER:HB2	2.02	0.59
1:A:435:VAL:HG13	1:A:435:VAL:O	2.03	0.59
1:D:108:TYR:HE1	1:D:119:VAL:HG21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ARG:NH2	1:D:138:VAL:HG12	2.17	0.59
1:A:368:VAL:HG13	1:A:369:GLY:N	2.16	0.59
1:A:291:MSE:HE2	1:A:360:SER:CB	2.32	0.59
1:C:262:MSE:O	1:C:265:THR:HB	2.03	0.59
1:A:383:VAL:HG12	1:A:383:VAL:O	2.03	0.59
1:C:305:GLU:O	1:C:306:ASN:HB2	2.03	0.59
1:C:232:MSE:HG2	1:C:290:TRP:HH2	1.66	0.59
1:B:224:PRO:CD	1:B:225:GLU:OE1	2.45	0.59
1:A:383:VAL:CG1	1:A:383:VAL:O	2.51	0.58
1:A:360:SER:O	1:A:363:THR:HB	2.03	0.58
1:B:302:HIS:CD2	1:B:311:THR:OG1	2.56	0.58
1:C:398:LEU:HD23	1:C:419:PRO:HB3	1.86	0.58
1:A:413:LEU:HD23	1:A:416:MSE:HE2	1.84	0.58
1:C:138:VAL:O	1:C:141:SER:HB3	2.03	0.58
1:B:134:ASP:C	1:B:134:ASP:OD1	2.42	0.58
1:A:368:VAL:CG1	1:A:369:GLY:N	2.67	0.58
1:C:350:GLN:CD	1:C:350:GLN:H	2.07	0.57
1:C:204:ARG:CG	1:C:208:MSE:HE2	2.34	0.57
1:C:397:MSE:HE1	1:C:432:MSE:CE	2.33	0.57
1:A:295:LYS:HE3	1:A:299:ASP:OD2	2.04	0.57
1:A:245:ASN:ND2	1:A:437:ASN:OD1	2.36	0.57
1:D:126:GLU:HB3	1:D:128:LEU:HD13	1.87	0.57
1:A:442:HIS:CD2	1:A:444:GLU:H	2.22	0.57
1:B:344:MSE:SE	1:B:440:ILE:CD1	3.02	0.57
1:A:190:LYS:NZ	1:A:198:ASP:CG	2.57	0.57
1:C:128:LEU:O	1:C:129:ALA:HB2	2.04	0.57
1:A:126:GLU:CD	1:A:165:ASN:HD21	2.07	0.57
1:C:186:GLU:CG	1:C:208:MSE:HE1	2.28	0.57
1:C:373:MSE:CE	1:C:393:TYR:CD2	2.83	0.57
1:A:126:GLU:OE1	1:A:165:ASN:ND2	2.34	0.57
1:C:265:THR:HG23	1:C:267:PHE:HD2	1.70	0.56
1:B:183:ASN:C	1:B:183:ASN:OD1	2.43	0.56
1:B:231:LEU:O	1:B:234:SER:CB	2.54	0.56
1:B:155:VAL:CG2	1:B:182:THR:HG23	2.36	0.56
1:D:103:GLY:HA2	1:D:314:CYS:SG	2.45	0.56
1:B:400:ILE:HG22	1:B:401:THR:HG23	1.87	0.56
1:A:150:HIS:HD2	1:A:295:LYS:HZ2	1.54	0.56
1:C:397:MSE:CE	1:C:432:MSE:HE1	2.36	0.56
1:B:112:CYS:SG	1:B:114:PRO:HD2	2.45	0.56
1:C:75:ILE:HD13	1:C:75:ILE:N	2.20	0.55
1:C:339:ARG:NH2	1:C:353:ALA:HB3	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:TYR:CE1	1:D:119:VAL:HG21	2.42	0.55
1:C:99:ILE:CD1	1:C:123:LEU:HD13	2.35	0.55
1:C:88:ILE:HG12	1:C:164:PRO:HB3	1.89	0.55
1:B:241:ASP:HA	1:B:246:ARG:HG2	1.89	0.55
1:B:386:THR:HG22	1:B:389:GLU:HB2	1.89	0.55
1:D:363:THR:HG23	1:D:368:VAL:HG12	1.88	0.54
1:A:58:THR:HG23	1:A:61:GLU:CB	2.35	0.54
1:A:291:MSE:CE	1:A:360:SER:HB3	2.36	0.54
1:B:386:THR:HG22	1:B:389:GLU:CB	2.37	0.54
1:A:363:THR:HG22	1:A:364:GLU:N	2.21	0.54
1:A:265:THR:HG22	1:A:267:PHE:N	2.15	0.54
1:A:371:PHE:CE1	1:A:422:ILE:HD11	2.42	0.54
1:A:320:PHE:O	1:A:334:THR:HA	2.07	0.54
1:A:240:GLY:O	1:A:246:ARG:HD3	2.07	0.54
1:D:131:ASP:OD2	1:D:134:ASP:OD1	2.26	0.54
1:B:383:VAL:O	1:B:383:VAL:CG1	2.55	0.54
1:A:244:HIS:HD1	1:A:363:THR:HG21	1.72	0.54
1:C:63:ILE:HD11	1:C:473:ILE:HD12	1.90	0.54
1:B:444:GLU:CB	1:B:447:ILE:HD12	2.38	0.54
1:C:466:LEU:O	1:C:470:VAL:HG13	2.08	0.54
1:B:435:VAL:CG1	1:B:435:VAL:O	2.56	0.53
1:D:196:ALA:N	1:D:446:GLY:HA2	2.22	0.53
1:A:315:ARG:NH2	1:A:358:GLY:O	2.39	0.53
1:D:364:GLU:OE1	1:D:436:ILE:HA	2.08	0.53
1:A:413:LEU:HB3	1:A:416:MSE:HG2	1.91	0.53
1:C:373:MSE:CE	1:C:393:TYR:HB2	2.39	0.53
1:B:59:LEU:O	1:B:62:LYS:N	2.42	0.53
1:C:109:GLU:CD	1:C:109:GLU:H	2.12	0.53
1:C:245:ASN:HD21	1:C:438:THR:HA	1.74	0.53
1:C:232:MSE:HG2	1:C:290:TRP:CH2	2.44	0.53
1:B:444:GLU:HB2	1:B:447:ILE:HD12	1.91	0.53
1:C:150:HIS:HD2	1:C:295:LYS:HZ3	1.55	0.53
1:B:240:GLY:O	1:B:246:ARG:HD3	2.09	0.53
1:B:386:THR:HG23	1:B:388:ALA:N	2.24	0.53
1:B:269:ARG:HG2	2:B:2:PEG:O4	2.09	0.52
1:B:435:VAL:HG13	1:B:435:VAL:O	2.08	0.52
1:D:150:HIS:HD2	1:D:295:LYS:HZ2	1.57	0.52
1:B:298:LEU:HD23	1:B:362:ILE:HG13	1.91	0.52
1:B:372:ALA:O	1:B:373:MSE:C	2.48	0.52
1:C:339:ARG:NH2	1:C:350:GLN:O	2.42	0.52
1:C:350:GLN:NE2	1:C:350:GLN:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:GLU:OE2	1:D:163:SER:HB2	2.10	0.52
1:C:197:ASN:OD1	1:C:197:ASN:N	2.43	0.52
1:C:363:THR:HG22	1:C:364:GLU:N	2.24	0.52
1:D:134:ASP:O	1:D:138:VAL:N	2.25	0.52
1:B:360:SER:O	1:B:363:THR:HB	2.10	0.52
1:C:198:ASP:HB2	1:C:200:SER:OG	2.10	0.52
1:C:259:THR:N	1:C:260:PRO:HD2	2.25	0.51
1:A:100:LEU:O	1:A:161:VAL:HA	2.10	0.51
1:A:473:ILE:O	1:A:473:ILE:HG22	2.09	0.51
1:A:307:SER:OG	1:A:309:ILE:HG12	2.10	0.51
1:D:430:THR:CG2	1:D:432:MSE:N	2.74	0.51
1:D:413:LEU:HB3	1:D:416:MSE:HG2	1.92	0.51
1:A:130:LYS:HB2	1:A:130:LYS:NZ	2.25	0.51
1:B:211:VAL:HG22	1:B:212:LEU:N	2.25	0.51
1:C:264:GLN:NE2	1:D:273:LYS:HD2	2.25	0.51
1:D:397:MSE:SE	1:D:432:MSE:HE1	2.60	0.51
1:D:322:ILE:HG12	1:D:461:VAL:HG13	1.92	0.51
1:C:103:GLY:HA2	1:C:314:CYS:SG	2.50	0.51
1:C:442:HIS:CD2	1:C:444:GLU:H	2.29	0.51
1:A:363:THR:CG2	1:A:364:GLU:N	2.74	0.51
1:D:392:ASN:ND2	1:D:396:GLU:OE2	2.44	0.51
1:B:244:HIS:HB2	1:B:363:THR:HG21	1.93	0.51
1:B:364:GLU:OE1	1:B:370:GLY:N	2.39	0.51
1:C:155:VAL:O	1:C:182:THR:HG22	2.10	0.50
1:A:244:HIS:ND1	1:A:363:THR:HG21	2.26	0.50
1:B:55:ASN:O	1:B:56:ALA:C	2.49	0.50
1:C:115:MSE:O	1:C:119:VAL:HG13	2.10	0.50
1:A:190:LYS:HZ1	1:A:198:ASP:CG	2.15	0.50
1:A:351:GLU:O	1:A:443:LYS:HE3	2.11	0.50
1:C:100:LEU:O	1:C:161:VAL:HA	2.11	0.50
1:B:231:LEU:O	1:B:234:SER:HB2	2.10	0.50
1:C:265:THR:CG2	1:C:266:ASP:N	2.73	0.50
1:A:78:LYS:HD3	1:A:174:GLU:OE1	2.12	0.50
1:C:242:GLU:O	1:C:368:VAL:HG13	2.12	0.50
1:D:430:THR:HG23	1:D:432:MSE:HB2	1.91	0.49
1:B:117:GLY:O	1:B:197:ASN:ND2	2.44	0.49
1:B:340:VAL:HB	1:B:440:ILE:CG2	2.32	0.49
1:B:88:ILE:HA	1:B:94:MSE:HG2	1.94	0.49
1:A:185:SER:C	1:A:186:GLU:O	2.49	0.49
1:B:163:SER:OG	1:B:166:MSE:HE3	2.12	0.49
1:D:207:TRP:O	1:D:211:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:NH1	1:B:350:GLN:OE1	2.46	0.49
1:D:268:SER:OG	1:D:271:GLN:HG3	2.12	0.49
1:B:340:VAL:CB	1:B:440:ILE:HG22	2.34	0.49
1:B:58:THR:OG1	1:B:59:LEU:N	2.41	0.49
1:D:322:ILE:HG12	1:D:461:VAL:CG1	2.41	0.49
1:D:115:MSE:O	1:D:119:VAL:HG13	2.13	0.49
1:D:105:PRO:O	1:D:106:ILE:CG2	2.58	0.49
1:D:134:ASP:N	1:D:134:ASP:OD1	2.30	0.49
1:B:383:VAL:HG12	1:B:383:VAL:O	2.12	0.49
1:D:156:GLY:H	1:D:359:ASP:HB2	1.78	0.49
1:D:120:GLN:HB3	1:D:132:LEU:HD22	1.95	0.49
1:C:430:THR:HG22	1:C:432:MSE:H	1.74	0.49
1:C:138:VAL:O	1:C:141:SER:N	2.46	0.49
1:A:233:LEU:C	1:A:233:LEU:CD1	2.80	0.49
1:D:412:VAL:HG13	1:D:413:LEU:HD13	1.94	0.49
1:C:273:LYS:HE2	1:C:277:GLU:OE1	2.13	0.49
1:D:99:ILE:HD13	1:D:161:VAL:HG13	1.95	0.49
1:B:340:VAL:HG11	1:B:438:THR:HG23	1.94	0.49
1:A:58:THR:CG2	1:A:61:GLU:CB	2.91	0.48
1:A:244:HIS:HB2	1:A:363:THR:HG21	1.95	0.48
1:B:58:THR:OG1	1:B:61:GLU:HG2	2.13	0.48
1:C:271:GLN:O	1:C:275:VAL:HG23	2.13	0.48
1:C:472:THR:HG23	1:C:472:THR:O	2.12	0.48
1:C:233:LEU:HD13	1:C:243:CYS:SG	2.53	0.48
1:A:58:THR:HG22	1:A:61:GLU:OE1	2.13	0.48
1:C:265:THR:CG2	1:C:267:PHE:H	2.24	0.48
1:C:208:MSE:HA	1:C:212:LEU:HB2	1.94	0.48
1:C:138:VAL:CG2	1:C:139:ALA:N	2.75	0.48
1:B:211:VAL:O	1:B:214:PRO:HD2	2.13	0.48
1:A:245:ASN:HD21	1:A:438:THR:CA	2.20	0.48
1:D:327:ILE:HD13	1:D:333:PHE:CZ	2.48	0.48
1:D:246:ARG:HB2	1:D:379:ILE:HG22	1.96	0.48
1:C:440:ILE:HG12	1:C:451:GLY:C	2.33	0.48
1:D:232:MSE:HA	1:D:235:GLN:NE2	2.29	0.48
1:D:364:GLU:H	1:D:364:GLU:HG2	1.24	0.48
1:A:233:LEU:CD1	1:A:237:LEU:HD13	2.44	0.48
1:B:118:ALA:HB1	1:B:161:VAL:HG21	1.95	0.48
1:C:411:PRO:HB3	1:C:415:PHE:CE1	2.49	0.48
1:C:184:LEU:HD23	1:C:212:LEU:HD13	1.95	0.48
1:A:265:THR:CG2	1:A:267:PHE:CD2	2.94	0.48
1:C:108:TYR:HB2	1:C:146:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:MSE:CE	1:D:432:MSE:CE	2.91	0.47
1:D:360:SER:O	1:D:363:THR:HB	2.14	0.47
1:D:442:HIS:HD2	1:D:444:GLU:N	2.10	0.47
1:D:327:ILE:HD13	1:D:333:PHE:HZ	1.79	0.47
1:D:245:ASN:HD21	1:D:437:ASN:C	2.18	0.47
1:C:437:ASN:HA	1:C:454:LEU:HD12	1.96	0.47
1:B:150:HIS:HD2	1:B:295:LYS:NZ	2.12	0.47
1:B:262:MSE:HE1	1:B:275:VAL:HG11	1.96	0.47
1:B:339:ARG:HH11	1:B:339:ARG:HB3	1.79	0.47
1:C:115:MSE:HE1	1:C:316:ASN:HB2	1.96	0.47
1:C:204:ARG:O	1:C:208:MSE:HG3	2.14	0.47
1:B:262:MSE:O	1:B:265:THR:HB	2.14	0.47
1:D:386:THR:HG23	1:D:389:GLU:H	1.80	0.47
1:B:262:MSE:HE1	1:B:275:VAL:CG1	2.44	0.47
1:C:158:MSE:O	1:C:358:GLY:HA2	2.14	0.47
1:D:352:ASP:HB3	1:D:442:HIS:CE1	2.50	0.47
1:A:83:GLY:HA2	1:A:220:MSE:HG3	1.96	0.47
1:D:96:GLU:OE2	1:D:96:GLU:HA	2.15	0.47
1:C:363:THR:HG22	1:C:364:GLU:OE2	2.15	0.46
1:D:124:VAL:HG21	1:D:132:LEU:HD23	1.97	0.46
1:B:58:THR:OG1	1:B:61:GLU:CG	2.63	0.46
1:C:298:LEU:HD23	1:C:362:ILE:CD1	2.46	0.46
1:C:229:LEU:HD12	1:C:229:LEU:HA	1.60	0.46
1:D:401:THR:HB	1:D:420:THR:O	2.15	0.46
1:C:342:GLY:HA3	1:C:452:ALA:O	2.15	0.46
1:A:473:ILE:O	1:A:474:ASN:CB	2.63	0.46
1:B:340:VAL:HG13	1:B:455:THR:HB	1.97	0.46
1:A:150:HIS:CD2	1:A:295:LYS:NZ	2.83	0.46
1:B:392:ASN:O	1:B:396:GLU:HG3	2.14	0.46
1:C:367:GLY:O	1:C:418:ILE:HB	2.15	0.46
1:C:396:GLU:HG3	1:C:397:MSE:HE2	1.97	0.46
1:C:397:MSE:HE2	1:C:432:MSE:HE1	1.97	0.46
1:C:192:LEU:HD22	1:C:205:LEU:HD11	1.98	0.46
1:A:194:PHE:CZ	1:A:449:MSE:HB2	2.50	0.46
1:B:265:THR:CG2	1:B:267:PHE:H	2.19	0.46
1:C:323:ARG:HD2	1:C:332:TRP:CH2	2.51	0.46
1:B:349:THR:HG23	1:B:352:ASP:OD1	2.16	0.46
1:B:118:ALA:CB	1:B:161:VAL:HG21	2.46	0.46
1:B:370:GLY:O	1:B:373:MSE:HB2	2.16	0.45
1:C:284:TYR:OH	1:C:291:MSE:CE	2.64	0.45
1:D:169:HIS:CE1	1:D:184:LEU:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:MSE:HE3	1:B:248:VAL:HB	1.98	0.45
1:C:138:VAL:HG23	1:C:139:ALA:N	2.31	0.45
1:B:108:TYR:HE1	1:B:119:VAL:HG21	1.79	0.45
1:C:420:THR:HG22	1:C:421:GLY:N	2.31	0.45
1:B:61:GLU:O	1:B:64:GLN:N	2.50	0.45
1:B:132:LEU:HD21	1:B:197:ASN:OD1	2.16	0.45
1:B:190:LYS:HE2	1:B:198:ASP:OD2	2.16	0.45
1:D:432:MSE:HB3	1:D:432:MSE:HE2	1.67	0.45
1:A:158:MSE:CB	1:A:193:ARG:HG3	2.46	0.45
1:B:208:MSE:HA	1:B:212:LEU:HB3	1.97	0.45
1:C:158:MSE:H	1:C:158:MSE:HE2	1.81	0.45
1:B:186:GLU:HG3	1:B:186:GLU:H	1.63	0.45
1:C:215:LEU:HD21	1:C:262:MSE:HE3	1.97	0.45
1:C:212:LEU:HD22	1:C:216:LEU:CD2	2.46	0.45
1:C:430:THR:HG21	1:C:432:MSE:HB2	1.98	0.45
1:C:163:SER:OG	1:C:166:MSE:HE3	2.17	0.45
1:A:244:HIS:HD1	1:A:363:THR:CG2	2.30	0.45
1:A:218:ASP:O	1:A:221:THR:HB	2.17	0.45
1:B:423:ASP:C	1:B:423:ASP:OD2	2.56	0.45
1:C:269:ARG:HG2	2:D:3:PEG:O4	2.17	0.45
1:C:327:ILE:HD13	1:C:333:PHE:CE2	2.52	0.45
1:D:265:THR:HG23	1:D:267:PHE:N	2.29	0.44
1:A:58:THR:HG22	1:A:61:GLU:HB2	1.95	0.44
1:B:262:MSE:CE	1:B:275:VAL:HG11	2.47	0.44
1:C:116:LYS:O	1:C:119:VAL:HG22	2.17	0.44
1:D:246:ARG:HB2	1:D:379:ILE:CG2	2.48	0.44
1:D:88:ILE:HA	1:D:94:MSE:HG2	2.00	0.44
1:B:342:GLY:HA3	1:B:452:ALA:O	2.16	0.44
1:B:265:THR:HG23	1:B:266:ASP:N	2.32	0.44
1:A:371:PHE:CE1	1:A:422:ILE:CD1	3.00	0.44
1:B:59:LEU:C	1:B:61:GLU:N	2.70	0.44
1:D:100:LEU:O	1:D:161:VAL:HA	2.17	0.44
1:A:265:THR:HG21	1:A:267:PHE:HD2	1.80	0.44
1:A:321:GLY:HA2	1:A:333:PHE:O	2.18	0.44
1:D:135:ALA:CA	1:D:138:VAL:HG22	2.40	0.44
1:A:412:VAL:HG13	1:A:413:LEU:HD13	1.99	0.44
1:D:402:THR:O	1:D:403:LYS:HB3	2.17	0.44
1:A:265:THR:HG21	1:A:267:PHE:CD2	2.53	0.44
1:B:386:THR:CG2	1:B:389:GLU:N	2.64	0.44
1:C:163:SER:HB2	1:C:164:PRO:HD2	1.99	0.44
1:B:83:GLY:C	1:B:170:ILE:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:HIS:HD2	1:B:311:THR:OG1	1.99	0.44
1:C:264:GLN:HE21	1:D:273:LYS:HD2	1.83	0.44
1:A:440:ILE:HG13	1:A:452:ALA:HA	2.00	0.44
1:A:345:PHE:HB3	1:A:346:ALA:H	1.35	0.44
1:D:71:VAL:HA	1:D:74:ILE:HD12	1.99	0.44
1:A:108:TYR:CZ	1:A:116:LYS:HD3	2.53	0.43
1:D:69:GLU:HA	1:D:69:GLU:OE1	2.18	0.43
1:D:59:LEU:HD23	1:D:60:TYR:N	2.33	0.43
1:C:84:PHE:CD2	1:C:216:LEU:HB3	2.54	0.43
1:B:259:THR:HB	1:B:260:PRO:HD3	2.01	0.43
1:D:112:CYS:SG	1:D:114:PRO:HD2	2.57	0.43
1:B:315:ARG:NE	1:B:356:ASP:OD2	2.48	0.43
1:C:473:ILE:O	1:C:474:ASN:CG	2.57	0.43
1:A:382:LEU:O	1:A:382:LEU:HG	2.18	0.43
1:B:190:LYS:HD3	1:B:198:ASP:OD2	2.18	0.43
1:B:442:HIS:HD2	1:B:444:GLU:N	2.03	0.43
1:C:298:LEU:HD23	1:C:362:ILE:HD11	2.01	0.43
1:D:59:LEU:HD23	1:D:59:LEU:C	2.38	0.43
1:A:424:VAL:O	1:A:428:LEU:HD22	2.18	0.43
1:C:373:MSE:CE	1:C:393:TYR:CB	2.97	0.43
1:B:272:LEU:HD12	1:B:272:LEU:HA	1.88	0.43
1:A:324:VAL:O	1:A:327:ILE:HG22	2.19	0.43
1:D:108:TYR:HB2	1:D:146:PHE:CE2	2.53	0.43
1:A:190:LYS:HZ3	1:A:198:ASP:CG	2.22	0.43
1:D:350:GLN:CA	1:D:350:GLN:NE2	2.79	0.43
1:D:216:LEU:HA	1:D:216:LEU:HD12	1.84	0.43
1:D:98:THR:O	1:D:164:PRO:HD3	2.19	0.43
1:C:265:THR:CG2	1:C:267:PHE:HD2	2.31	0.42
1:D:376:ALA:O	1:D:379:ILE:HG12	2.19	0.42
1:D:244:HIS:CD2	1:D:244:HIS:C	2.92	0.42
1:C:374:ALA:HB1	1:C:391:LEU:HD23	2.01	0.42
1:D:265:THR:CG2	1:D:267:PHE:H	2.28	0.42
1:B:67:ASN:O	1:B:71:VAL:HG12	2.18	0.42
1:D:361:ALA:C	1:D:363:THR:N	2.70	0.42
1:D:241:ASP:OD1	1:D:246:ARG:O	2.37	0.42
1:C:428:LEU:HA	1:C:428:LEU:HD12	1.63	0.42
1:A:126:GLU:CD	1:A:165:ASN:ND2	2.73	0.42
1:D:420:THR:HG22	1:D:421:GLY:N	2.33	0.42
1:D:91:MSE:HB3	1:D:91:MSE:HE2	1.93	0.42
1:D:242:GLU:C	1:D:242:GLU:OE1	2.57	0.42
1:A:447:ILE:CG2	1:A:448:GLY:N	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:MSE:SE	1:B:440:ILE:HD12	2.70	0.42
1:D:361:ALA:C	1:D:363:THR:H	2.23	0.42
1:A:371:PHE:HE1	1:A:422:ILE:CD1	2.31	0.42
1:A:90:VAL:HG13	1:A:181:PHE:CE1	2.55	0.42
1:C:255:VAL:HG22	1:C:279:LEU:HD13	2.02	0.42
1:D:397:MSE:HE2	1:D:432:MSE:HE1	1.97	0.42
1:C:129:ALA:O	1:C:130:LYS:C	2.57	0.42
1:C:363:THR:CG2	1:C:369:GLY:HA3	2.50	0.42
1:C:438:THR:HG23	1:C:439:ALA:O	2.20	0.42
1:D:150:HIS:CD2	1:D:295:LYS:NZ	2.82	0.42
1:B:400:ILE:O	1:B:400:ILE:CG2	2.67	0.42
1:D:392:ASN:HD22	1:D:392:ASN:C	2.22	0.42
1:C:241:ASP:OD1	1:C:246:ARG:HG2	2.20	0.42
1:C:254:LEU:HA	1:C:254:LEU:HD23	1.93	0.42
1:D:198:ASP:O	1:D:202:VAL:HG23	2.20	0.42
1:B:184:LEU:N	1:B:184:LEU:HD12	2.35	0.41
1:A:317:GLY:HA2	1:A:356:ASP:O	2.20	0.41
1:D:123:LEU:HD13	1:D:138:VAL:HG23	2.01	0.41
1:A:58:THR:HG23	1:A:61:GLU:H	1.85	0.41
1:C:155:VAL:CG2	1:C:182:THR:HG23	2.47	0.41
1:B:315:ARG:HD2	1:B:320:PHE:CE1	2.55	0.41
1:B:88:ILE:HD13	1:B:88:ILE:O	2.21	0.41
1:B:79:PRO:O	1:B:229:LEU:HB2	2.21	0.41
1:C:199:GLN:NE2	1:C:203:ASP:OD1	2.53	0.41
1:B:100:LEU:HD23	1:B:100:LEU:N	2.36	0.41
1:B:368:VAL:HG13	1:B:369:GLY:N	2.35	0.41
1:D:155:VAL:O	1:D:182:THR:CG2	2.65	0.41
1:B:134:ASP:OD1	1:B:134:ASP:O	2.39	0.41
1:B:187:GLN:HE22	1:B:285:PHE:N	2.18	0.41
1:D:232:MSE:HE1	1:D:257:ALA:HB2	2.01	0.41
1:B:150:HIS:CD2	1:B:295:LYS:NZ	2.88	0.41
1:A:225:GLU:CD	1:A:225:GLU:H	2.23	0.41
1:A:466:LEU:O	1:A:470:VAL:HG13	2.20	0.41
1:C:190:LYS:HD2	1:C:190:LYS:HA	1.95	0.41
1:C:69:GLU:HG2	1:C:304:VAL:HG11	2.02	0.41
1:A:269:ARG:HG2	2:B:2:PEG:H21	2.02	0.41
1:A:364:GLU:H	1:A:364:GLU:HG2	1.50	0.41
1:C:239:MSE:HE3	1:D:248:VAL:HG12	2.02	0.41
1:B:462:PHE:O	1:B:465:ALA:HB3	2.21	0.41
1:D:119:VAL:O	1:D:123:LEU:HG	2.20	0.41
1:C:157:SER:HB2	1:C:291:MSE:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ILE:HG12	1:B:451:GLY:O	2.21	0.40
1:C:126:GLU:CB	1:C:128:LEU:HD12	2.51	0.40
1:A:307:SER:HG	1:A:309:ILE:HG12	1.85	0.40
1:A:217:HIS:HD2	1:A:218:ASP:OD2	2.03	0.40
1:B:211:VAL:CG2	1:B:212:LEU:N	2.84	0.40
1:B:199:GLN:O	1:B:200:SER:C	2.59	0.40
1:D:134:ASP:O	1:D:135:ALA:C	2.58	0.40
1:A:84:PHE:HA	1:A:168:VAL:O	2.22	0.40
1:C:136:ASP:O	1:C:137:ARG:C	2.58	0.40
1:C:456:ASN:CB	1:C:457:PRO:HD2	2.49	0.40
1:D:103:GLY:O	1:D:148:PRO:HB3	2.21	0.40
1:B:88:ILE:HB	1:B:164:PRO:HB3	2.02	0.40
1:D:383:VAL:O	1:D:383:VAL:HG13	2.22	0.40
1:D:363:THR:HG22	1:D:364:GLU:N	2.37	0.40
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.98	0.40
1:A:251:SER:O	1:A:255:VAL:HG13	2.21	0.40
1:D:307:SER:HB3	1:D:325:SER:HB3	2.02	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	418/421 (99%)	392 (94%)	22 (5%)	4 (1%)	19	34
1	B	419/421 (100%)	380 (91%)	33 (8%)	6 (1%)	14	24
1	C	419/421 (100%)	390 (93%)	27 (6%)	2 (0%)	34	55
1	D	417/421 (99%)	386 (93%)	27 (6%)	4 (1%)	19	34
All	All	1673/1684 (99%)	1548 (92%)	109 (6%)	16 (1%)	19	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	ILE
1	A	346	ALA
1	B	57	PRO
1	B	373	MSE
1	C	129	ALA
1	B	473	ILE
1	D	345	PHE
1	A	198	ASP
1	A	345	PHE
1	B	56	ALA
1	C	130	LYS
1	D	373	MSE
1	B	60	TYR
1	D	198	ASP
1	B	113	GLY
1	D	368	VAL

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	336/317 (106%)	302 (90%)	34 (10%)	9 17
1	B	337/317 (106%)	287 (85%)	50 (15%)	4 7
1	C	337/317 (106%)	295 (88%)	42 (12%)	6 10
1	D	335/317 (106%)	295 (88%)	40 (12%)	6 12
All	All	1345/1268 (106%)	1179 (88%)	166 (12%)	6 11

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	64	GLN
1	A	90	VAL
1	A	123	LEU
1	A	128	LEU
1	A	165	ASN

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Mol	Chain	Res	Type
1	A	184	LEU
1	A	193	ARG
1	A	202	VAL
1	A	211	VAL
1	A	216	LEU
1	A	221	THR
1	A	229	LEU
1	A	233	LEU
1	A	242	GLU
1	A	254	LEU
1	A	255	VAL
1	A	265	THR
1	A	272	LEU
1	A	281	SER
1	A	315	ARG
1	A	324	VAL
1	A	327	ILE
1	A	339	ARG
1	A	349	THR
1	A	363	THR
1	A	364	GLU
1	A	386	THR
1	A	387	VAL
1	A	396	GLU
1	A	413	LEU
1	A	428	LEU
1	A	429	GLU
1	A	454	LEU
1	B	58	THR
1	B	59	LEU
1	B	61	GLU
1	B	64	GLN
1	B	78	LYS
1	B	88	ILE
1	B	99	ILE
1	B	123	LEU
1	B	182	THR
1	B	190	LYS
1	B	191	VAL
1	B	199	GLN
1	B	205	LEU
1	B	209	ARG

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Mol	Chain	Res	Type
1	B	211	VAL
1	B	216	LEU
1	B	229	LEU
1	B	234	SER
1	B	237	LEU
1	B	242	GLU
1	B	254	LEU
1	B	255	VAL
1	B	265	THR
1	B	269	ARG
1	B	272	LEU
1	B	273	LYS
1	B	298	LEU
1	B	315	ARG
1	B	327	ILE
1	B	339	ARG
1	B	341	ILE
1	B	349	THR
1	B	350	GLN
1	B	355	LEU
1	B	364	GLU
1	B	368	VAL
1	B	386	THR
1	B	387	VAL
1	B	392	ASN
1	B	397	MSE
1	B	400	ILE
1	B	413	LEU
1	B	420	THR
1	B	428	LEU
1	B	429	GLU
1	B	433	LEU
1	B	436	ILE
1	B	438	THR
1	B	450	ILE
1	B	461	VAL
1	C	69	GLU
1	C	75	ILE
1	C	88	ILE
1	C	90	VAL
1	C	96	GLU
1	C	123	LEU

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Mol	Chain	Res	Type
1	C	147	SER
1	C	182	THR
1	C	190	LYS
1	C	197	ASN
1	C	199	GLN
1	C	211	VAL
1	C	212	LEU
1	C	215	LEU
1	C	216	LEU
1	C	225	GLU
1	C	229	LEU
1	C	237	LEU
1	C	242	GLU
1	C	254	LEU
1	C	265	THR
1	C	270	GLU
1	C	272	LEU
1	C	277	GLU
1	C	281	SER
1	C	298	LEU
1	C	315	ARG
1	C	349	THR
1	C	350	GLN
1	C	351	GLU
1	C	363	THR
1	C	368	VAL
1	C	413	LEU
1	C	416	MSE
1	C	428	LEU
1	C	429	GLU
1	C	430	THR
1	C	438	THR
1	C	454	LEU
1	C	461	VAL
1	C	470	VAL
1	C	472	THR
1	D	99	ILE
1	D	110	ASN
1	D	147	SER
1	D	182	THR
1	D	184	LEU
1	D	191	VAL

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Mol	Chain	Res	Type
1	D	193	ARG
1	D	211	VAL
1	D	215	LEU
1	D	216	LEU
1	D	229	LEU
1	D	233	LEU
1	D	237	LEU
1	D	241	ASP
1	D	242	GLU
1	D	252	THR
1	D	254	LEU
1	D	255	VAL
1	D	265	THR
1	D	269	ARG
1	D	272	LEU
1	D	315	ARG
1	D	323	ARG
1	D	349	THR
1	D	350	GLN
1	D	363	THR
1	D	364	GLU
1	D	382	LEU
1	D	383	VAL
1	D	392	ASN
1	D	400	ILE
1	D	403	LYS
1	D	413	LEU
1	D	416	MSE
1	D	425	LEU
1	D	430	THR
1	D	433	LEU
1	D	454	LEU
1	D	456	ASN
1	D	474	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	65	GLN
1	A	150	HIS
1	A	165	ASN

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Mol	Chain	Res	Type
1	A	187	GLN
1	A	217	HIS
1	A	235	GLN
1	A	245	ASN
1	A	442	HIS
1	A	463	ASN
1	B	76	GLN
1	B	150	HIS
1	B	199	GLN
1	B	302	HIS
1	B	442	HIS
1	B	463	ASN
1	C	76	GLN
1	C	120	GLN
1	C	150	HIS
1	C	187	GLN
1	C	245	ASN
1	C	264	GLN
1	C	350	GLN
1	C	442	HIS
1	C	463	ASN
1	D	150	HIS
1	D	235	GLN
1	D	302	HIS
1	D	350	GLN
1	D	392	ASN
1	D	442	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	PEG	B	1	-	6,6,6	0.40	0	5,5,5	0.51	0
2	PEG	B	2	-	6,6,6	0.65	0	5,5,5	0.36	0
2	PEG	C	4	-	6,6,6	0.48	0	5,5,5	0.36	0
2	PEG	D	3	-	6,6,6	0.56	0	5,5,5	0.19	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	PEG	B	1	-	-	0/4/4/4	0/0/0/0
2	PEG	B	2	-	-	0/4/4/4	0/0/0/0
2	PEG	C	4	-	-	0/4/4/4	0/0/0/0
2	PEG	D	3	-	-	0/4/4/4	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	PEG	3	0
2	D	3	PEG	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	400/421 (95%)	-0.01	5 (1%) 79 82	44, 55, 66, 78	0
1	B	401/421 (95%)	0.19	10 (2%) 61 65	47, 55, 63, 88	0
1	C	401/421 (95%)	0.14	9 (2%) 65 69	47, 54, 63, 80	0
1	D	399/421 (94%)	0.21	10 (2%) 61 65	47, 55, 64, 73	0
All	All	1601/1684 (95%)	0.13	34 (2%) 67 71	44, 55, 64, 88	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	SER	4.8
1	C	54	SER	3.9
1	D	59	LEU	3.5
1	D	88	ILE	3.5
1	D	474	ASN	3.4
1	C	55	ASN	3.2
1	B	55	ASN	3.1
1	A	240	GLY	2.9
1	B	346	ALA	2.9
1	D	347	GLY	2.9
1	B	133	ALA	2.8
1	D	348	TYR	2.8
1	A	346	ALA	2.8
1	C	139	ALA	2.8
1	A	347	GLY	2.6
1	C	132	LEU	2.6
1	D	393	TYR	2.6
1	D	206	ILE	2.6
1	B	474	ASN	2.5
1	D	222	PHE	2.4
1	B	60	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	99	ILE	2.4
1	D	470	VAL	2.4
1	C	135	ALA	2.3
1	B	240	GLY	2.3
1	A	474	ASN	2.2
1	B	56	ALA	2.2
1	B	349	THR	2.2
1	C	137	ARG	2.1
1	C	211	VAL	2.1
1	B	347	GLY	2.1
1	D	240	GLY	2.0
1	A	348	TYR	2.0
1	C	474	ASN	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
2	PEG	C	4	7/7	0.89	0.22	2.29	73,75,75,75	0
2	PEG	B	1	7/7	0.95	0.11	-1.26	59,61,64,66	0
2	PEG	D	3	7/7	0.84	0.24	-	83,84,84,84	0
2	PEG	B	2	7/7	0.80	0.35	-	77,78,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.