Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 07:45 pm BST

PDB ID	:	5OTB
Title	:	Structure of caprine serum albumin in P1 space group
Authors	:	Talaj, J.A.; Bujacz, A.; Bujacz, G.
Deposited on	:	2017-08-21
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

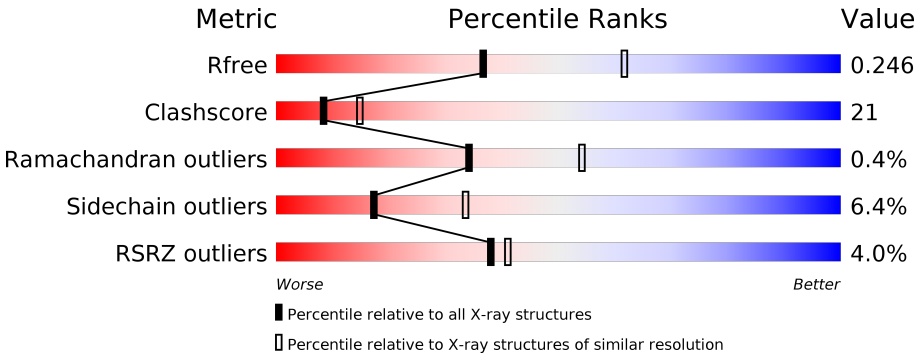
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	583	3% 58% 38% .
1	B	583	5% 58% 40% .
1	C	583	5% 60% 36% .
1	D	583	3% 61% 36% .

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
3	PRO	A	602	-	-	X	-
3	PRO	B	602	-	-	X	-
3	PRO	D	602	-	-	X	-

2 Entry composition

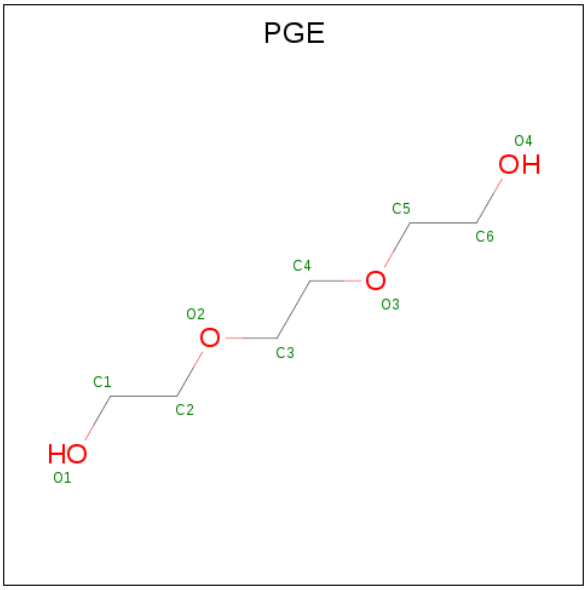
There are 5 unique types of molecules in this entry. The entry contains 19131 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4628	2922	777	890	39			
1	B	581	Total	C	N	O	S	0	0	0
			4627	2922	777	889	39			
1	C	581	Total	C	N	O	S	0	0	0
			4628	2922	777	890	39			
1	D	581	Total	C	N	O	S	0	1	0
			4634	2927	778	890	39			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			10	6	4			
2	B	1	Total	C	O		0	0
			10	6	4			

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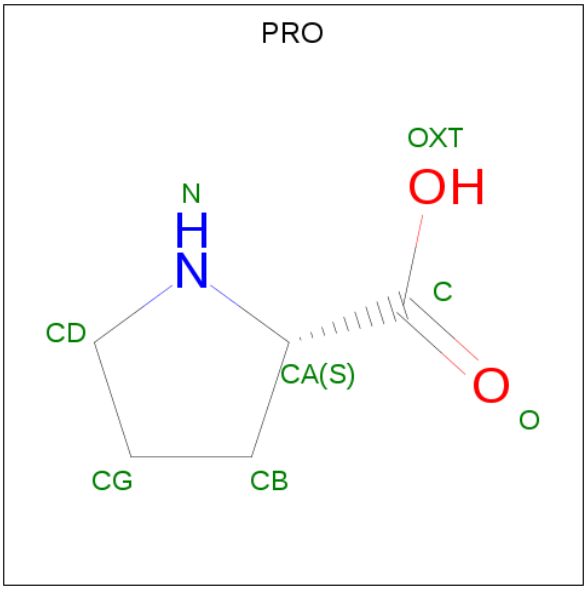
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 10 6 4	0	0

- Molecule 3 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 8 5 1 2	0	0
3	A	1	Total C N O 8 5 1 2	0	0
3	B	1	Total C N O 8 5 1 2	0	0
3	B	1	Total C N O 8 5 1 2	0	0
3	C	1	Total C N O 8 5 1 2	0	0
3	C	1	Total C N O 8 5 1 2	0	0
3	C	1	Total C N O 8 5 1 2	0	0
3	D	1	Total C N O 8 5 1 2	0	0
3	D	1	Total C N O 8 5 1 2	0	0
3	D	1	Total C N O 8 5 1 2	0	0

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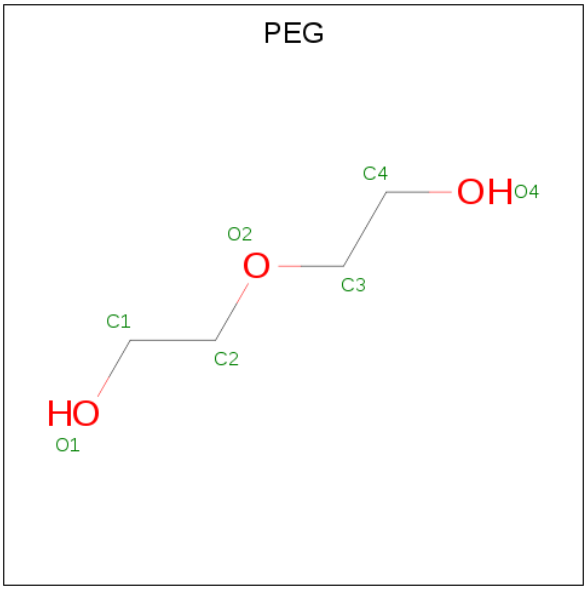
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is water.

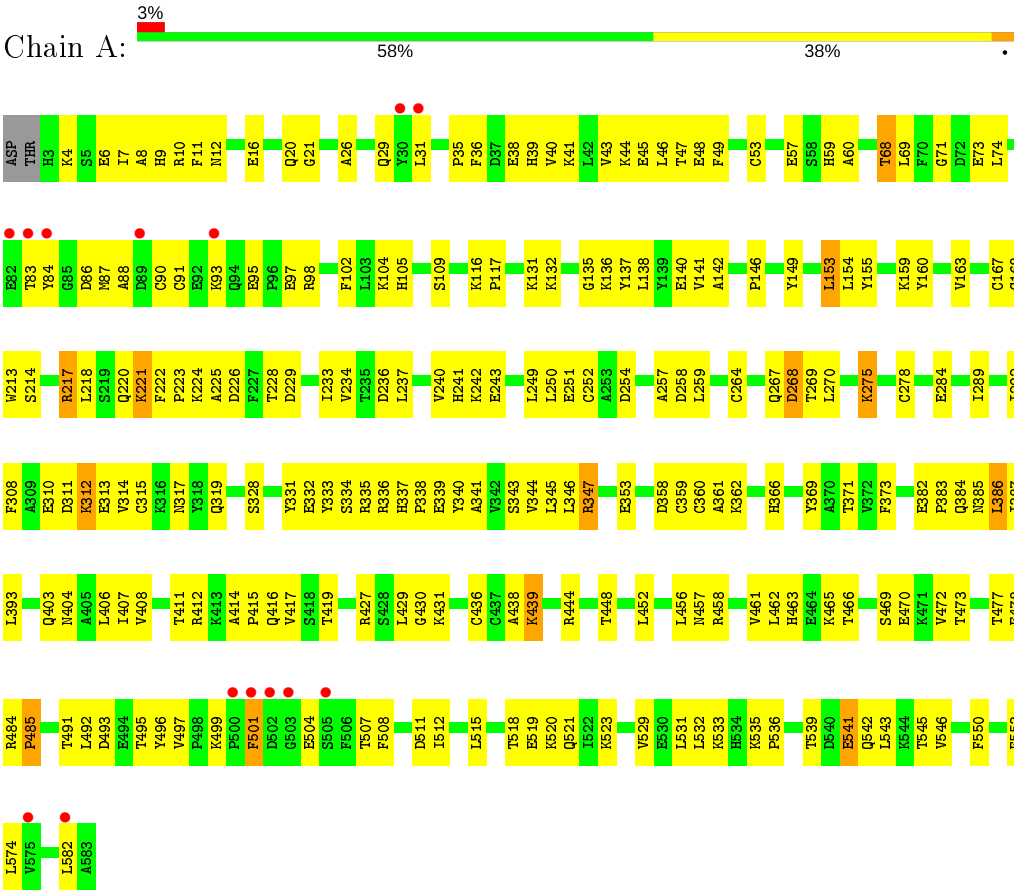
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	124	Total	O	0	0
			124	124		
5	C	124	Total	O	0	0
			124	124		
5	D	126	Total	O	0	0
			126	126		

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

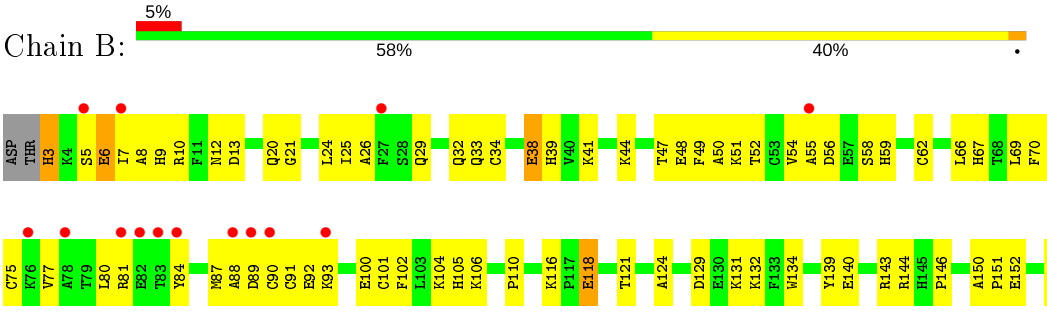
- Molecule 1: Albumin

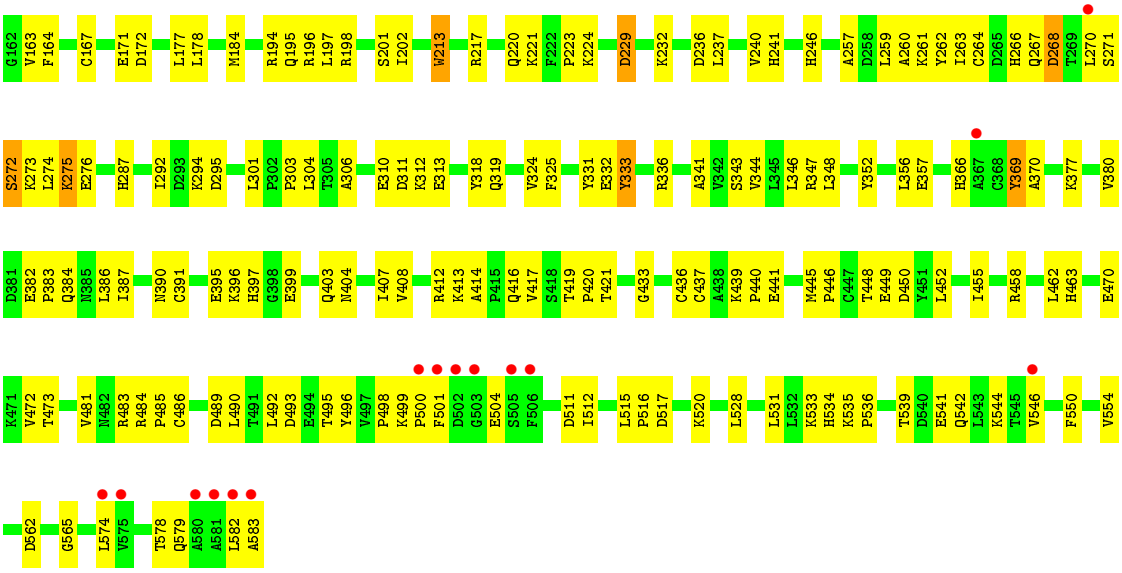
Chain A:



- Molecule 1: Albumin

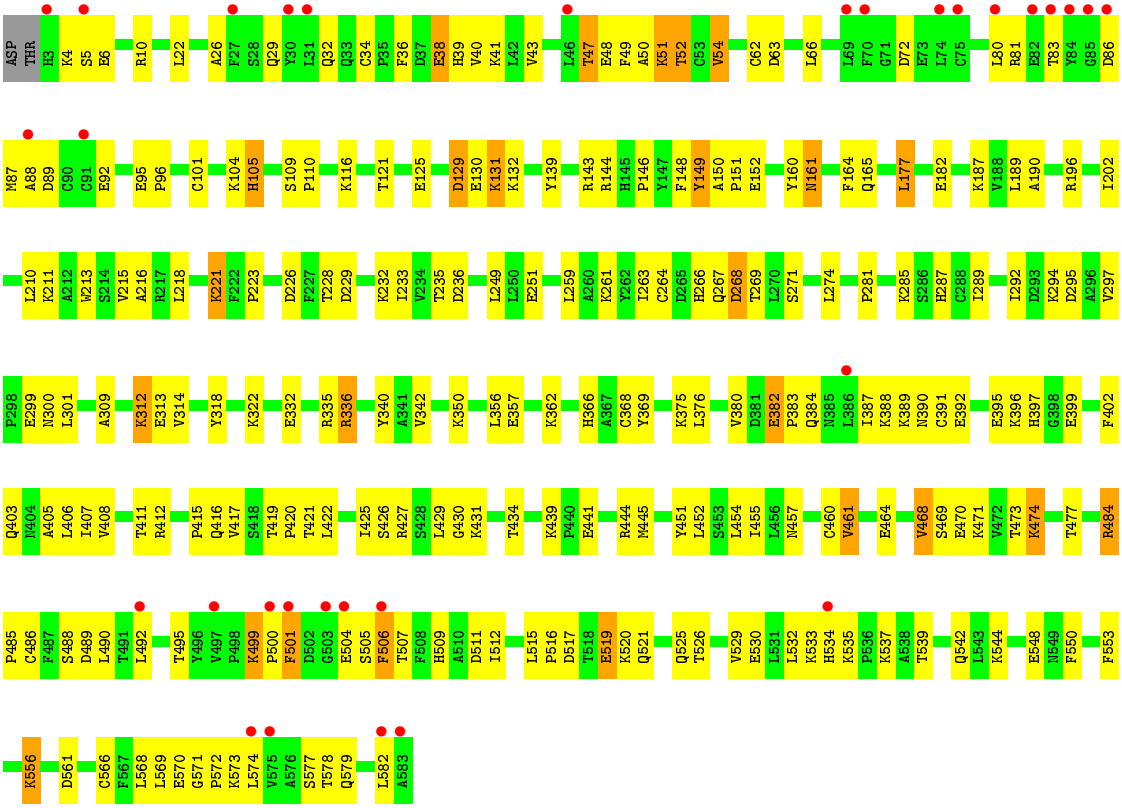
Chain B:





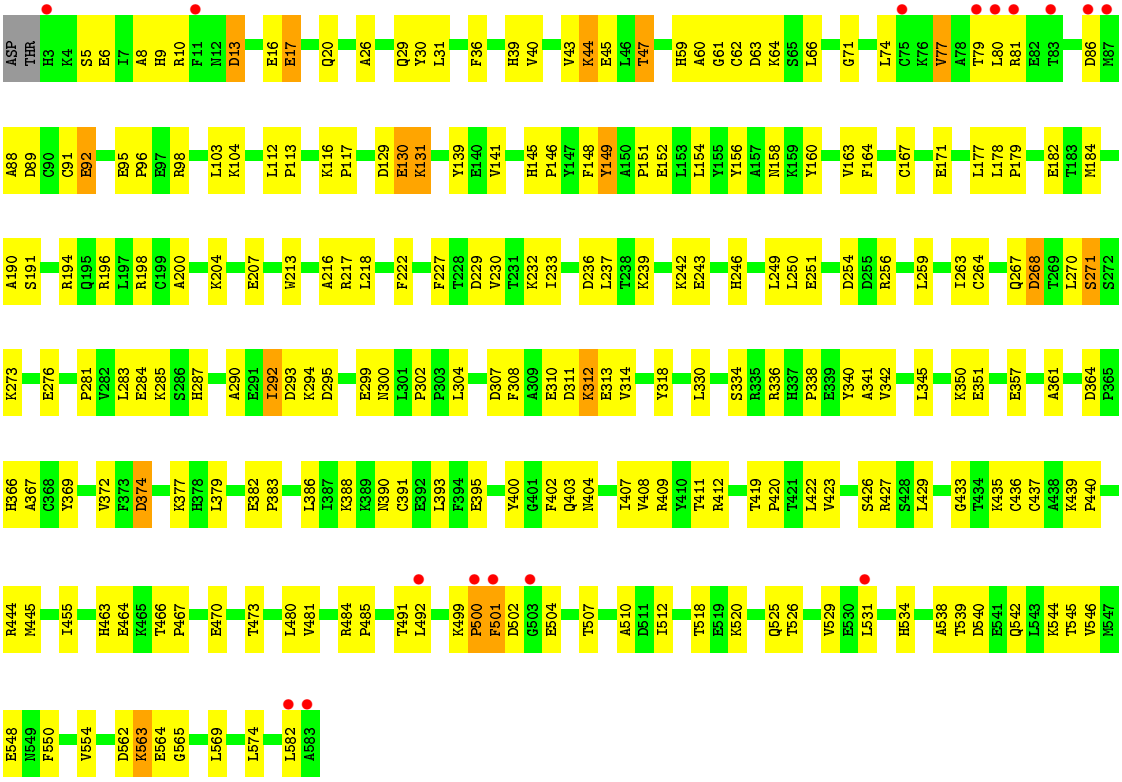
- Molecule 1: Albumin

Chain C:



- Molecule 1: Albumin

Chain D:


ASP THR H3 K4 S5 E6 I7 A8 H9 R10 F11 N12 D13 E16 E17 Q20 A26 Q29 Y30 L31 F36 H39 V40 V43 K44 E45 L46 T47 H59 A60 G61 C62 D63 K64 S65 L66 G71 L74 C75 K76 V77 A78 T79 L80 R81 E82 T83 D86 M87
A88 D89 C90 C91 E92 E95 P96 E97 R98 L103 K104 L112 P113 K116 P117 D129 E130 K131 Y139 E140 V141 H145 P146 Y147 F148 Y149 A150 P151 E152 L153 L154 Y155 Y156 A157 N158 K159 Y160 V163 F164 C167 E171 L177 L178 P179 E182 T183 M184
A190 S191 R194 Q195 R196 L197 R198 C199 A200 K204 E207 W213 A216 R217 L218 F222 F227 T228 D229 V230 T231 K232 I233 D236 L237 T238 K239 K242 E243 H246 L249 L250 E251 D254 D255 R256 L259 I263 C264 Q267 D268 T269 L270 S271 S272
K273 E276 P281 V282 L283 E284 K285 S286 H287 A290 E291 I292 D293 K294 D295 E299 N300 L301 P302 P303 L304 D307 F308 A309 E310 D311 K312 E313 V314 Y318 L330 S334 R335 R336 H337 P338 E339 Y340 A341 V342 L345 K350 E351 E357 A361 D364 P365
H366 A367 C368 Y369 V372 F373 D374 K377 H378 L379 E382 P383 L386 I387 K388 K389 N390 C391 E392 L393 F394 E395 Y400 G401 F402 Q403 N404 I407 V408 R409 Y410 T411 R412 T419 P420 T421 L422 V423 S426 R427 S428 L429 G433 T434 K435 C436 C437 A438 K439 P440
R444 M445 I455 H463 E464 K465 T466 P467 E470 T473 L480 V481 R484 P485 T491 L492 K499 P500 F501 D502 Q503 E504 T507 A510 D511 I512 T518 E519 K520 Q525 T526 V529 E530 L531 H534 A538 T539 D540 E541 Q542 L543 K544 T545 V546 M547
E548 N549 F550 V554 D562 K563 E564 G565 L569 L574 L582 A583

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.75Å 80.93Å 110.53Å 90.01° 75.90° 72.22°	Depositor
Resolution (Å)	40.00 – 2.50 39.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-2.50) 98.2 (39.47-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.197 , 0.246 0.198 , 0.246	Depositor DCC
R_{free} test set	1707 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19131	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PGE

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	0.92	0/4724	1.03	0/6376
1	B	0.93	0/4723	1.04	0/6374
1	C	0.90	0/4724	1.00	0/6376
1	D	0.96	0/4733	1.04	0/6387
All	All	0.93	0/18904	1.03	0/25513

There are no bond length outliers.

There are no bond angle outliers.

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	4628	0	4537	210	0
1	B	4627	0	4537	200	1
1	C	4628	0	4537	191	1
1	D	4634	0	4550	177	2
2	A	10	0	14	1	0
2	B	10	0	14	1	0
2	C	10	0	14	0	0
3	A	16	0	14	12	0
3	B	16	0	14	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	24	0	21	6	0
3	D	32	0	28	15	0
4	C	7	0	10	1	0
4	D	7	0	10	2	0
5	A	108	0	0	6	0
5	B	124	0	0	5	0
5	C	124	0	0	9	0
5	D	126	0	0	10	0
All	All	19131	0	18300	773	2

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 21.

All (773) 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:498:PRO:O	1:B:500:PRO:HD3	1.31	1.26
1:A:116:LYS:HE3	1:B:116:LYS:HE3	1.28	1.08
1:C:86:ASP:O	1:C:89:ASP:HB2	1.60	1.02
1:B:539:THR:HB	1:B:542:GLN:HB2	1.44	0.99
1:C:499:LYS:HG3	1:C:500:PRO:HD2	1.45	0.98
1:D:382:GLU:HB2	1:D:383:PRO:HD3	1.47	0.96
1:B:56:ASP:HB3	1:B:59:HIS:HB2	1.47	0.96
1:B:498:PRO:HB3	1:B:536:PRO:HG2	1.49	0.95
1:C:517:ASP:HA	1:C:520:LYS:HD2	1.46	0.95
1:B:484:ARG:HB3	1:B:485:PRO:HD3	1.45	0.95
1:A:415:PRO:HD2	1:A:416:GLN:NE2	1.83	0.94
1:D:390:ASN:HB3	4:D:601:PEG:H42	1.49	0.93
1:C:569:LEU:HD22	1:C:570:GLU:HG2	1.50	0.93
1:A:80:LEU:HB2	1:A:88:ALA:HB2	1.52	0.91
1:C:383:PRO:O	1:C:387:ILE:HD13	1.70	0.90
1:C:29:GLN:HG2	1:C:146:PRO:HA	1.55	0.88
1:B:74:LEU:O	1:B:77:VAL:HB	1.74	0.86
1:D:89:ASP:O	1:D:92:GLU:HB2	1.75	0.86
1:C:457:ASN:O	1:C:461:VAL:HG13	1.77	0.84
1:C:504:GLU:O	1:C:507:THR:HG22	1.79	0.83
1:B:498:PRO:O	1:B:500:PRO:CD	2.24	0.82
1:D:88:ALA:O	1:D:91:CYS:HB2	1.80	0.82
1:B:131:LYS:HD2	3:B:602:PRO:CB	2.09	0.82
1:C:460:CYS:O	1:C:464:GLU:HB2	1.81	0.81
1:B:50:ALA:O	1:B:54:VAL:HG23	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:HG3	3:C:603:PRO:HG3	1.64	0.80
1:C:451:TYR:HA	1:C:454:LEU:HD12	1.64	0.79
1:D:310:GLU:HA	1:D:366:HIS:NE2	1.98	0.79
1:D:81:ARG:HG2	1:D:88:ALA:HB3	1.63	0.79
1:A:98:ARG:HD3	1:A:102:PHE:HE2	1.47	0.78
1:A:71:GLY:HA2	1:A:74:LEU:HD12	1.65	0.78
1:A:213:TRP:CD1	3:A:602:PRO:N	2.50	0.78
1:B:131:LYS:HD2	3:B:602:PRO:HB3	1.65	0.78
1:A:26:ALA:HB2	1:A:249:LEU:HD12	1.66	0.78
1:D:341:ALA:HB2	1:D:445:MET:HG2	1.66	0.78
1:A:213:TRP:HD1	3:A:602:PRO:N	1.81	0.78
1:D:463:HIS:HE1	1:D:473:THR:HB	1.49	0.78
1:B:32:GLN:O	1:B:143:ARG:NE	2.18	0.77
1:B:275:LYS:HE3	1:B:275:LYS:O	1.84	0.77
1:D:264:CYS:O	1:D:267:GLN:HG2	1.85	0.77
1:A:38:GLU:OE2	1:A:41:LYS:HE3	1.86	0.76
1:C:511:ASP:O	1:C:515:LEU:HG	1.85	0.76
1:C:556:LYS:HE3	1:C:570:GLU:OE2	1.86	0.76
1:C:5:SER:HB3	1:C:62:CYS:O	1.85	0.76
1:D:382:GLU:HB2	1:D:383:PRO:CD	2.16	0.75
1:A:264:CYS:O	1:A:267:GLN:HG3	1.87	0.75
1:C:561:ASP:OD1	1:D:435:LYS:HD3	1.85	0.75
1:D:525:GLN:O	1:D:529:VAL:HG23	1.87	0.75
1:A:550:PHE:CD1	1:A:574:LEU:HD21	2.22	0.74
1:C:382:GLU:HB3	1:C:383:PRO:HD2	1.68	0.74
1:A:484:ARG:N	1:A:485:PRO:HD2	2.01	0.74
1:A:463:HIS:CD2	1:A:472:VAL:HG12	2.23	0.74
1:B:100:GLU:O	1:B:104:LYS:HG3	1.87	0.74
1:C:419:THR:HG21	1:C:526:THR:HG23	1.67	0.74
1:C:289:ILE:O	1:C:292:ILE:HG22	1.88	0.74
1:D:86:ASP:O	1:D:89:ASP:OD1	2.06	0.73
1:B:390:ASN:ND2	2:B:601:PGE:H32	2.04	0.73
1:D:550:PHE:CE2	1:D:574:LEU:HD21	2.23	0.73
1:A:87:MET:O	1:A:90:CYS:HB2	1.88	0.73
1:B:531:LEU:HD11	1:B:582:LEU:HD11	1.69	0.73
1:A:213:TRP:HZ3	1:A:217:ARG:HD2	1.53	0.73
1:B:220:GLN:O	1:B:223:PRO:HD3	1.89	0.72
1:C:318:TYR:OH	1:C:357:GLU:OE1	2.07	0.72
1:A:217:ARG:HG3	1:A:218:LEU:N	2.05	0.71
1:A:98:ARG:HD3	1:A:102:PHE:CE2	2.26	0.71
1:C:471:LYS:HD3	1:C:490:LEU:HD22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:LYS:HG3	1:C:500:PRO:CD	2.20	0.71
1:C:51:LYS:O	1:C:54:VAL:HG12	1.90	0.71
1:D:531:LEU:HD11	1:D:546:VAL:HG11	1.72	0.71
1:A:214:SER:HA	1:A:217:ARG:HG2	1.73	0.70
1:A:87:MET:HE2	1:A:105:HIS:HB2	1.72	0.70
1:A:497:VAL:CG1	1:A:499:LYS:HE2	2.21	0.70
1:C:268:ASP:N	1:C:268:ASP:OD2	2.21	0.69
1:D:550:PHE:CD2	1:D:574:LEU:HD21	2.27	0.69
1:B:34:CYS:HB2	1:B:39:HIS:CE1	2.26	0.69
1:B:44:LYS:O	1:B:48:GLU:HG2	1.93	0.69
1:C:569:LEU:CD2	1:C:570:GLU:HG2	2.23	0.69
1:C:89:ASP:O	1:C:92:GLU:HB3	1.93	0.69
1:B:386:LEU:HD12	1:B:387:ILE:HD13	1.73	0.69
1:D:131:LYS:HE3	3:D:602:PRO:CA	2.23	0.69
1:A:412:ARG:HB3	1:A:492:LEU:HG	1.74	0.69
1:B:484:ARG:HB3	1:B:485:PRO:CD	2.22	0.69
1:C:407:ILE:HD12	1:C:525:GLN:HG2	1.74	0.68
1:A:116:LYS:HE3	1:B:116:LYS:CE	2.15	0.68
1:C:419:THR:CG2	1:C:526:THR:HG23	2.21	0.68
1:A:404:ASN:O	1:A:408:VAL:HG23	1.93	0.68
1:B:77:VAL:HG12	1:B:77:VAL:O	1.93	0.68
1:A:463:HIS:HE1	1:A:469:SER:H	1.42	0.68
1:B:213:TRP:HZ3	1:B:217:ARG:HD2	1.58	0.68
1:B:156:TYR:O	1:B:184:MET:HE1	1.94	0.67
1:C:399:GLU:O	1:C:403:GLN:HG3	1.92	0.67
1:C:121:THR:O	1:C:125:GLU:HG3	1.95	0.67
1:D:26:ALA:HB2	1:D:249:LEU:HD12	1.75	0.67
1:D:390:ASN:CB	4:D:601:PEG:H42	2.25	0.67
1:B:67:HIS:HE1	1:B:246:HIS:HE1	1.41	0.67
1:B:264:CYS:O	1:B:267:GLN:HG2	1.95	0.66
1:A:95:GLU:OE1	1:A:98:ARG:HD2	1.95	0.66
1:C:259:LEU:O	1:C:263:ILE:HG13	1.95	0.66
1:A:80:LEU:CB	1:A:88:ALA:HB2	2.26	0.66
1:B:272:SER:HB2	1:B:295:ASP:OD1	1.95	0.66
1:B:131:LYS:HD2	3:B:602:PRO:HB2	1.76	0.66
1:B:71:GLY:O	1:B:75:CYS:HB2	1.96	0.66
1:B:262:TYR:C	1:B:262:TYR:CD2	2.69	0.66
1:B:539:THR:CB	1:B:542:GLN:HB2	2.24	0.66
1:C:38:GLU:O	1:C:41:LYS:HG2	1.95	0.65
1:C:439:LYS:O	1:C:444:ARG:NH2	2.30	0.65
1:D:156:TYR:O	1:D:184:MET:HE3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:ARG:HD3	1:D:492:LEU:HD22	1.78	0.65
1:B:413:LYS:HE2	1:B:490:LEU:O	1.96	0.65
1:B:332:GLU:OE1	1:B:336:ARG:NH2	2.29	0.65
1:A:390:ASN:HB3	2:A:601:PGE:H2	1.79	0.65
1:A:39:HIS:O	1:A:43:VAL:HG23	1.97	0.64
1:C:150:ALA:HB3	1:C:151:PRO:HD3	1.79	0.64
1:A:539:THR:HG22	1:A:541:GLU:H	1.62	0.64
1:B:562:ASP:OD2	1:B:565:GLY:HA3	1.96	0.64
1:A:497:VAL:HG11	1:A:499:LYS:HE2	1.79	0.64
1:A:135:GLY:HA2	1:A:138:LEU:HD12	1.80	0.64
1:B:414:ALA:HB1	1:B:417:VAL:HG23	1.81	0.63
1:D:302:PRO:O	1:D:336:ARG:NH1	2.30	0.63
1:B:29:GLN:HE21	1:B:146:PRO:HA	1.64	0.63
1:B:246:HIS:ND1	1:B:246:HIS:O	2.32	0.63
1:C:530:GLU:HA	1:C:533:LYS:HB2	1.81	0.63
1:D:304:LEU:O	1:D:308:PHE:HD2	1.81	0.63
1:C:4:LYS:O	1:C:63:ASP:HA	1.99	0.63
1:B:152:GLU:OE2	1:B:287:HIS:ND1	2.25	0.63
1:D:36:PHE:HB2	1:D:139:TYR:CE2	2.34	0.62
1:C:417:VAL:HG13	5:C:765:HOH:O	1.98	0.62
1:D:470:GLU:HA	1:D:473:THR:HG22	1.81	0.62
1:B:458:ARG:CZ	1:B:462:LEU:HD21	2.30	0.62
1:B:84:TYR:HB2	1:B:87:MET:HB2	1.81	0.62
1:A:492:LEU:HD12	1:A:492:LEU:H	1.64	0.62
1:A:315:CYS:O	1:A:319:GLN:HG3	2.00	0.62
1:D:466:THR:OG1	1:D:466:THR:O	2.12	0.62
1:D:412:ARG:HB3	1:D:492:LEU:HD22	1.81	0.61
1:A:473:THR:O	1:A:477:THR:OG1	2.09	0.61
1:A:29:GLN:HG2	1:A:146:PRO:HA	1.83	0.61
1:B:515:LEU:HD22	1:B:516:PRO:HD2	1.82	0.61
1:B:550:PHE:O	1:B:554:VAL:HG23	1.99	0.61
1:D:369:TYR:O	1:D:372:VAL:HG12	2.00	0.61
1:B:66:LEU:HA	1:B:69:LEU:HD12	1.82	0.61
1:D:31:LEU:HD11	1:D:74:LEU:HD22	1.80	0.61
1:D:131:LYS:HE3	3:D:602:PRO:CB	2.29	0.61
1:C:87:MET:HE3	1:C:105:HIS:HB2	1.82	0.61
1:A:312:LYS:O	1:A:312:LYS:HD2	2.00	0.61
1:B:89:ASP:O	1:B:92:GLU:HB2	2.00	0.61
1:C:5:SER:CB	1:C:62:CYS:O	2.48	0.61
1:B:66:LEU:O	1:B:70:PHE:HD2	1.84	0.60
1:C:569:LEU:O	1:C:572:PRO:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:PRO:HA	1:A:386:LEU:HD23	1.84	0.60
1:A:427:ARG:HG2	1:A:427:ARG:HH11	1.65	0.60
1:B:56:ASP:CB	1:B:59:HIS:HB2	2.28	0.60
1:C:266:HIS:HB3	1:C:269:THR:OG1	2.00	0.60
1:C:202:ILE:HG13	1:C:210:LEU:HD22	1.83	0.60
3:D:604:PRO:HB3	5:D:817:HOH:O	2.00	0.60
1:A:77:VAL:O	1:A:80:LEU:HG	2.02	0.60
1:D:44:LYS:HD2	1:D:45:GLU:HG2	1.83	0.60
1:D:74:LEU:O	1:D:77:VAL:HB	2.02	0.60
1:A:87:MET:HE3	1:A:105:HIS:HB3	1.84	0.59
1:A:346:LEU:HD12	3:A:602:PRO:HG2	1.84	0.59
1:C:251:GLU:OE1	1:C:251:GLU:N	2.30	0.59
1:C:473:THR:O	1:C:477:THR:OG1	2.16	0.59
1:B:38:GLU:O	1:B:41:LYS:HG2	2.01	0.59
1:D:213:TRP:HB3	3:D:603:PRO:OXT	2.03	0.59
1:A:346:LEU:HD12	3:A:602:PRO:HB2	1.84	0.59
1:A:80:LEU:HB2	1:A:88:ALA:CB	2.31	0.59
1:C:515:LEU:HB3	1:C:519:GLU:HB2	1.85	0.59
1:D:31:LEU:HD11	1:D:74:LEU:CD2	2.32	0.59
1:A:532:LEU:HD21	1:A:543:LEU:HD11	1.85	0.58
1:A:10:ARG:NH1	1:A:254:ASP:OD2	2.37	0.58
1:A:214:SER:O	1:A:218:LEU:HB2	2.03	0.58
1:A:109:SER:HB3	1:A:465:LYS:NZ	2.19	0.58
1:A:550:PHE:HD1	1:A:574:LEU:HD21	1.65	0.58
1:C:226:ASP:HB3	1:C:228:THR:H	1.68	0.58
1:D:351:GLU:HG2	1:D:379:LEU:HD11	1.85	0.58
1:A:220:GLN:HG2	1:A:338:PRO:HA	1.86	0.58
1:A:539:THR:HB	1:A:542:GLN:HG3	1.85	0.58
1:B:273:LYS:HB2	1:B:292:ILE:HD11	1.86	0.58
1:C:403:GLN:HG2	1:C:430:GLY:HA3	1.84	0.58
1:A:207:GLU:OE1	1:A:242:LYS:HD3	2.04	0.57
1:A:59:HIS:CG	1:A:60:ALA:N	2.71	0.57
1:B:414:ALA:HB1	1:B:417:VAL:CG2	2.33	0.57
1:D:232:LYS:HE2	1:D:236:ASP:OD2	2.04	0.57
1:A:484:ARG:H	1:A:485:PRO:HD2	1.68	0.57
1:C:340:TYR:HA	1:C:445:MET:HE3	1.86	0.57
1:D:178:LEU:N	1:D:179:PRO:CD	2.66	0.57
1:D:152:GLU:OE2	1:D:287:HIS:ND1	2.30	0.57
1:A:457:ASN:O	1:A:461:VAL:HG13	2.04	0.57
1:D:167:CYS:HB3	1:D:177:LEU:HD12	1.87	0.57
1:D:29:GLN:HG2	1:D:146:PRO:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:GLU:CD	1:D:470:GLU:N	2.58	0.57
1:C:412:ARG:HG2	1:C:492:LEU:HD13	1.87	0.57
1:C:419:THR:HB	1:C:420:PRO:HD3	1.87	0.57
1:C:578:THR:HG22	1:C:579:GLN:HG3	1.85	0.57
1:C:501:PHE:HB3	1:C:579:GLN:NE2	2.20	0.57
1:B:301:LEU:HD12	1:B:336:ARG:HG3	1.85	0.57
1:B:408:VAL:HG13	1:B:412:ARG:NH1	2.20	0.57
1:A:93:LYS:HE3	1:A:97:GLU:HB3	1.85	0.56
1:C:553:PHE:HE1	1:C:570:GLU:HB2	1.69	0.56
1:A:87:MET:CE	1:A:105:HIS:HB2	2.33	0.56
1:B:387:ILE:HD12	1:B:448:THR:HG21	1.86	0.56
1:A:93:LYS:HE2	1:D:276:GLU:HG3	1.88	0.56
1:C:501:PHE:HD1	1:C:534:HIS:CE1	2.22	0.56
1:D:350:LYS:HD3	1:D:481:VAL:HG11	1.86	0.56
1:A:497:VAL:HG13	1:A:499:LYS:HE2	1.86	0.56
1:B:332:GLU:HB3	1:B:336:ARG:HH21	1.71	0.56
1:D:500:PRO:O	1:D:504:GLU:HG2	2.06	0.56
1:A:226:ASP:HB3	1:A:228:THR:H	1.70	0.56
1:A:313:GLU:O	1:A:317:ASN:OD1	2.24	0.56
1:B:412:ARG:O	1:B:492:LEU:HA	2.04	0.56
1:A:518:THR:O	1:A:521:GLN:HB2	2.06	0.56
1:B:6:GLU:OE2	1:B:10:ARG:NH2	2.39	0.56
1:D:393:LEU:HD23	1:D:402:PHE:CE1	2.39	0.56
1:A:462:LEU:O	1:A:465:LYS:HB3	2.06	0.56
1:D:218:LEU:O	1:D:218:LEU:HD23	2.06	0.56
1:D:463:HIS:CE1	1:D:473:THR:HB	2.38	0.56
1:D:540:ASP:O	1:D:544:LYS:HG2	2.06	0.56
1:A:249:LEU:O	1:A:252:CYS:HB3	2.06	0.56
1:C:573:LYS:O	1:C:577:SER:HB3	2.07	0.55
1:D:393:LEU:HD23	1:D:402:PHE:HE1	1.70	0.55
1:B:263:ILE:HG23	1:B:270:LEU:HD13	1.89	0.55
1:C:412:ARG:CG	1:C:492:LEU:HD13	2.35	0.55
1:D:294:LYS:HD2	1:D:338:PRO:HB3	1.86	0.55
1:A:159:LYS:HE2	1:A:284:GLU:OE1	2.07	0.55
1:C:271:SER:OG	1:C:295:ASP:HB2	2.07	0.55
1:D:263:ILE:HG23	1:D:270:LEU:HD13	1.88	0.55
1:D:429:LEU:HD23	1:D:455:ILE:HD13	1.87	0.55
1:A:346:LEU:HD12	3:A:602:PRO:CB	2.37	0.55
1:A:49:PHE:CE2	1:A:69:LEU:HD21	2.42	0.55
1:B:273:LYS:O	1:B:276:GLU:HB3	2.07	0.55
1:D:167:CYS:HB3	1:D:177:LEU:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ARG:NH1	1:B:81:ARG:HB3	2.22	0.55
1:C:390:ASN:HB3	3:C:604:PRO:HB3	1.88	0.55
1:B:528:LEU:O	1:B:531:LEU:HB3	2.07	0.55
1:C:501:PHE:CD2	1:C:501:PHE:N	2.71	0.55
1:A:214:SER:HB3	1:A:234:VAL:HG22	1.89	0.54
1:A:343:SER:HA	3:A:602:PRO:HG2	1.87	0.54
1:A:41:LYS:O	1:A:45:GLU:HG3	2.07	0.54
1:C:6:GLU:OE2	1:C:10:ARG:NH2	2.40	0.54
1:C:499:LYS:CG	1:C:500:PRO:HD2	2.28	0.54
1:D:131:LYS:HE3	3:D:602:PRO:HA	1.89	0.54
1:A:458:ARG:O	1:A:461:VAL:HG22	2.07	0.54
1:A:518:THR:HA	1:A:521:GLN:OE1	2.07	0.54
1:B:237:LEU:HD11	1:B:241:HIS:CE1	2.41	0.54
1:B:213:TRP:HA	1:B:346:LEU:HD11	1.90	0.54
1:B:578:THR:HG22	1:B:579:GLN:HG3	1.89	0.54
1:D:218:LEU:HD21	1:D:222:PHE:CD2	2.43	0.54
1:B:306:ALA:HA	1:B:310:GLU:HG3	1.89	0.54
1:B:448:THR:O	1:B:452:LEU:HG	2.07	0.54
1:A:187:LYS:HE2	5:A:743:HOH:O	2.08	0.54
1:B:470:GLU:HA	1:B:473:THR:HG22	1.90	0.54
1:D:500:PRO:O	1:D:504:GLU:CG	2.56	0.54
1:D:499:LYS:O	1:D:534:HIS:ND1	2.41	0.54
1:A:213:TRP:CZ3	1:A:217:ARG:HD2	2.39	0.54
1:C:431:LYS:O	1:C:434:THR:N	2.40	0.54
1:C:516:PRO:HG2	1:C:519:GLU:HG2	1.89	0.54
1:D:160:TYR:HB2	1:D:184:MET:HE1	1.89	0.54
1:A:458:ARG:CZ	1:A:462:LEU:HD21	2.38	0.54
1:B:535:LYS:HG3	1:B:582:LEU:HB3	1.90	0.54
1:C:416:GLN:O	1:C:468:VAL:HG21	2.08	0.54
1:C:484:ARG:HB3	1:C:485:PRO:HD3	1.89	0.54
1:A:87:MET:CE	1:A:105:HIS:CB	2.86	0.53
1:C:362:LYS:HD2	1:C:368:CYS:SG	2.47	0.53
1:A:419:THR:OG1	1:A:533:LYS:NZ	2.38	0.53
1:A:520:LYS:HE2	5:A:792:HOH:O	2.06	0.53
1:D:59:HIS:CG	1:D:60:ALA:H	2.25	0.53
1:B:5:SER:HB3	1:B:62:CYS:O	2.08	0.53
1:C:129:ASP:HB3	5:C:772:HOH:O	2.07	0.53
1:D:334:SER:OG	1:D:345:LEU:HD13	2.08	0.53
1:C:49:PHE:O	1:C:52:THR:HG22	2.08	0.53
1:D:470:GLU:N	1:D:470:GLU:OE1	2.37	0.53
1:D:499:LYS:NZ	5:D:710:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:TYR:OH	1:A:159:LYS:HE3	2.09	0.53
1:B:129:ASP:HB3	1:B:132:LYS:HB3	1.91	0.53
1:C:382:GLU:HB3	1:C:383:PRO:CD	2.36	0.53
1:D:391:CYS:O	1:D:395:GLU:HG2	2.08	0.53
1:A:343:SER:HA	3:A:602:PRO:CG	2.39	0.53
1:B:106:LYS:HG2	1:B:146:PRO:HB2	1.90	0.53
1:B:67:HIS:HE1	1:B:246:HIS:CE1	2.24	0.53
1:C:218:LEU:HD21	4:C:602:PEG:H42	1.91	0.53
1:C:309:ALA:O	1:C:369:TYR:HE1	1.91	0.53
1:C:419:THR:HG23	1:C:529:VAL:HG11	1.90	0.53
1:C:407:ILE:O	1:C:411:THR:OG1	2.18	0.53
1:A:382:GLU:O	1:A:385:ASN:HB2	2.07	0.53
1:A:511:ASP:O	1:A:515:LEU:HG	2.08	0.53
1:D:59:HIS:CG	1:D:60:ALA:N	2.77	0.53
1:B:259:LEU:O	1:B:263:ILE:HG13	2.08	0.53
1:B:8:ALA:O	1:B:12:ASN:ND2	2.42	0.52
1:B:463:HIS:HE1	1:B:473:THR:HB	1.74	0.52
1:D:484:ARG:HB3	1:D:485:PRO:HD3	1.91	0.52
1:D:467:PRO:HB2	3:D:605:PRO:HD3	1.91	0.52
1:A:492:LEU:H	1:A:492:LEU:CD1	2.22	0.52
1:B:56:ASP:O	1:B:59:HIS:N	2.36	0.52
1:C:427:ARG:HH11	1:C:427:ARG:HG2	1.73	0.52
1:B:102:PHE:O	1:B:105:HIS:N	2.39	0.52
1:C:149:TYR:CD1	1:C:151:PRO:HD2	2.45	0.52
1:C:211:LYS:O	1:C:215:VAL:HG23	2.09	0.52
1:C:221:LYS:HA	1:C:294:LYS:HG2	1.91	0.52
1:C:452:LEU:HD13	1:C:484:ARG:HG3	1.90	0.52
1:D:271:SER:OG	1:D:295:ASP:HB2	2.09	0.52
1:A:16:GLU:OE2	3:A:603:PRO:HG3	2.09	0.52
1:B:455:ILE:O	1:B:458:ARG:HB3	2.10	0.52
1:C:384:GLN:HA	1:C:384:GLN:OE1	2.09	0.52
1:C:486:CYS:O	1:C:489:ASP:HB2	2.09	0.52
1:D:243:GLU:OE2	1:D:251:GLU:HB3	2.09	0.52
1:A:332:GLU:OE1	1:A:336:ARG:NH1	2.43	0.52
1:C:148:PHE:CD1	1:C:149:TYR:N	2.78	0.52
1:A:16:GLU:O	1:A:20:GLN:HG3	2.08	0.52
1:C:407:ILE:HG13	1:C:426:SER:HB2	1.92	0.52
1:D:294:LYS:HE3	1:D:338:PRO:HB2	1.90	0.52
1:D:407:ILE:HG13	1:D:426:SER:HB2	1.90	0.52
1:B:301:LEU:HB3	1:B:336:ARG:NH1	2.25	0.52
1:B:399:GLU:O	1:B:403:GLN:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ILE:HG22	1:A:388:LYS:N	2.24	0.52
1:B:463:HIS:CE1	1:B:472:VAL:HG12	2.45	0.52
1:C:229:ASP:O	1:C:233:ILE:HG13	2.10	0.52
1:C:417:VAL:HB	1:C:422:LEU:HD21	1.92	0.52
1:B:266:HIS:O	1:B:270:LEU:HG	2.10	0.52
1:C:471:LYS:HA	1:C:474:LYS:HE2	1.91	0.52
1:C:86:ASP:O	1:C:89:ASP:CB	2.47	0.52
1:D:30:TYR:HE1	1:D:103:LEU:HD23	1.75	0.52
1:D:217:ARG:NH2	1:D:290:ALA:O	2.43	0.52
1:B:194:ARG:NH1	5:B:708:HOH:O	2.42	0.52
1:D:151:PRO:O	1:D:154:LEU:HB2	2.10	0.52
1:A:403:GLN:HG2	1:A:430:GLY:HA3	1.92	0.51
1:B:25:ILE:O	1:B:29:GLN:HG3	2.11	0.51
1:C:521:GLN:O	1:C:525:GLN:N	2.40	0.51
1:D:419:THR:HB	1:D:420:PRO:HD3	1.92	0.51
1:D:10:ARG:HG3	1:D:250:LEU:HB3	1.93	0.51
1:B:47:THR:O	1:B:51:LYS:HG3	2.10	0.51
1:D:207:GLU:OE1	1:D:242:LYS:HD3	2.09	0.51
1:B:33:GLN:N	1:B:84:TYR:OH	2.43	0.51
1:D:182:GLU:HG2	5:D:761:HOH:O	2.10	0.51
1:A:237:LEU:HG	1:A:241:HIS:CE1	2.45	0.51
1:A:479:SER:OG	1:A:481:VAL:HG12	2.11	0.51
1:C:264:CYS:O	1:C:267:GLN:HG2	2.10	0.51
1:D:20:GLN:HE21	1:D:47:THR:HG21	1.74	0.51
1:A:341:ALA:O	1:A:344:VAL:N	2.41	0.51
1:A:448:THR:O	1:A:452:LEU:HG	2.11	0.51
1:A:236:ASP:O	1:A:240:VAL:HG23	2.11	0.51
1:A:268:ASP:N	1:A:268:ASP:OD1	2.40	0.51
1:A:427:ARG:NH1	1:A:427:ARG:HG2	2.25	0.51
1:B:150:ALA:HB3	1:B:151:PRO:HD3	1.93	0.51
1:D:6:GLU:C	1:D:8:ALA:H	2.14	0.51
1:B:52:THR:O	1:B:56:ASP:N	2.32	0.51
1:D:6:GLU:OE2	1:D:10:ARG:NE	2.41	0.51
1:B:121:THR:O	1:B:124:ALA:HB3	2.11	0.51
1:D:190:ALA:O	1:D:191:SER:C	2.48	0.51
1:D:408:VAL:HG12	1:D:409:ARG:N	2.26	0.51
1:B:177:LEU:HD12	1:B:178:LEU:N	2.27	0.50
1:A:539:THR:HG22	1:A:541:GLU:N	2.26	0.50
1:B:140:GLU:O	1:B:144:ARG:HG3	2.11	0.50
1:C:50:ALA:O	1:C:52:THR:N	2.45	0.50
1:D:130:GLU:HG2	3:D:602:PRO:OXT	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:PHE:HZ	1:B:504:GLU:HG3	1.76	0.50
1:D:77:VAL:O	1:D:80:LEU:HG	2.11	0.50
1:A:11:PHE:CD1	1:A:11:PHE:C	2.85	0.50
1:A:226:ASP:HB2	1:A:229:ASP:H	1.76	0.50
1:A:484:ARG:N	1:A:485:PRO:CD	2.70	0.50
1:B:301:LEU:CD1	1:B:336:ARG:HG3	2.40	0.50
1:B:421:THR:HG23	1:B:462:LEU:HD12	1.94	0.50
1:A:153:LEU:HD12	1:A:153:LEU:O	2.12	0.50
1:A:419:THR:HG23	1:A:529:VAL:HG11	1.93	0.50
1:B:198:ARG:O	1:B:201:SER:HB2	2.12	0.50
1:A:59:HIS:CG	1:A:60:ALA:H	2.29	0.50
1:B:134:TRP:CD1	3:B:602:PRO:HD3	2.47	0.50
1:C:507:THR:HG23	1:C:509:HIS:HE1	1.76	0.50
1:C:511:ASP:N	1:C:511:ASP:OD1	2.45	0.50
1:C:571:GLY:N	1:C:572:PRO:HD2	2.26	0.50
1:B:81:ARG:HG3	1:B:88:ALA:CB	2.42	0.49
1:D:5:SER:HA	1:D:63:ASP:HA	1.93	0.49
1:D:216:ALA:HB2	1:D:330:LEU:HD11	1.94	0.49
1:D:311:ASP:OD1	1:D:312:LYS:N	2.45	0.49
1:D:9:HIS:ND1	1:D:9:HIS:O	2.45	0.49
1:B:534:HIS:NE2	1:B:579:GLN:HG2	2.27	0.49
1:C:332:GLU:OE1	1:C:336:ARG:NH2	2.44	0.49
1:C:50:ALA:C	1:C:52:THR:H	2.15	0.49
1:D:470:GLU:H	1:D:470:GLU:CD	2.15	0.49
1:A:341:ALA:HB3	1:A:344:VAL:HG23	1.94	0.49
1:C:216:ALA:HB3	1:C:342:VAL:HG13	1.94	0.49
1:C:427:ARG:NH1	1:C:427:ARG:HG2	2.27	0.49
1:D:281:PRO:O	1:D:285:LYS:HB2	2.12	0.49
1:A:46:LEU:HD13	1:A:73:GLU:OE1	2.12	0.49
1:B:333:TYR:OH	1:B:377:LYS:NZ	2.31	0.49
1:B:369:TYR:HD1	1:B:369:TYR:O	1.96	0.49
1:C:144:ARG:HH11	1:C:144:ARG:HG3	1.78	0.49
1:C:406:LEU:HD13	1:C:429:LEU:HB3	1.93	0.49
1:C:48:GLU:O	1:C:51:LYS:HB2	2.13	0.49
1:D:163:VAL:O	1:D:167:CYS:HB2	2.12	0.49
1:D:131:LYS:CE	3:D:602:PRO:HB2	2.42	0.49
1:B:304:LEU:HD11	1:B:333:TYR:HA	1.93	0.49
1:B:56:ASP:O	1:B:58:SER:N	2.46	0.49
1:A:415:PRO:HG2	1:A:496:TYR:CD2	2.46	0.49
1:C:32:GLN:HG2	1:C:143:ARG:O	2.12	0.49
1:B:52:THR:HA	1:B:55:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ARG:HB3	1:B:81:ARG:HH11	1.78	0.49
1:D:39:HIS:O	1:D:43:VAL:HG23	2.12	0.49
1:D:470:GLU:OE2	3:D:605:PRO:HG3	2.13	0.49
1:A:222:PHE:N	1:A:222:PHE:CD1	2.77	0.49
1:B:20:GLN:O	1:B:21:GLY:C	2.52	0.49
1:C:553:PHE:CE1	1:C:570:GLU:HB2	2.47	0.49
1:A:138:LEU:O	1:A:142:ALA:HB3	2.13	0.48
1:B:344:VAL:O	1:B:348:LEU:HG	2.12	0.48
1:B:318:TYR:OH	1:B:357:GLU:OE1	2.26	0.48
1:C:380:VAL:O	1:C:384:GLN:HG2	2.13	0.48
1:A:87:MET:HE3	1:A:105:HIS:CB	2.43	0.48
1:C:380:VAL:O	1:C:383:PRO:HG2	2.13	0.48
1:D:281:PRO:O	1:D:285:LYS:CB	2.61	0.48
1:A:346:LEU:HD12	3:A:602:PRO:CG	2.43	0.48
1:C:87:MET:CE	1:C:105:HIS:HB2	2.42	0.48
1:B:3:HIS:CD2	1:B:9:HIS:HB2	2.49	0.48
1:A:136:LYS:O	1:A:140:GLU:HG2	2.14	0.48
1:A:501:PHE:O	1:A:504:GLU:O	2.32	0.48
1:B:483:ARG:O	1:B:484:ARG:C	2.50	0.48
1:D:294:LYS:HD2	1:D:338:PRO:CB	2.43	0.48
1:A:31:LEU:HD11	1:A:74:LEU:HD23	1.95	0.48
1:A:473:THR:O	1:A:473:THR:HG22	2.14	0.48
1:B:229:ASP:N	1:B:229:ASP:OD1	2.45	0.48
1:B:221:LYS:HG2	1:B:292:ILE:HG23	1.96	0.48
1:D:283:LEU:O	1:D:284:GLU:C	2.51	0.48
1:D:400:TYR:O	1:D:403:GLN:HB2	2.14	0.48
1:A:84:TYR:HB2	1:A:87:MET:HB3	1.96	0.47
1:B:395:GLU:OE1	1:B:395:GLU:HA	2.13	0.47
1:B:271:SER:HB3	1:B:274:LEU:HG	1.96	0.47
1:B:535:LYS:HE2	1:B:583:ALA:HA	1.95	0.47
1:D:423:VAL:O	1:D:427:ARG:HG3	2.14	0.47
1:B:383:PRO:HA	1:B:386:LEU:HG	1.95	0.47
1:A:116:LYS:HE2	1:B:118:GLU:HG2	1.96	0.47
1:A:439:LYS:O	1:A:444:ARG:NH1	2.48	0.47
1:A:501:PHE:CE2	1:A:533:LYS:HD3	2.49	0.47
1:B:171:GLU:HG2	1:B:172:ASP:N	2.29	0.47
1:B:404:ASN:O	1:B:407:ILE:HB	2.15	0.47
1:C:407:ILE:CD1	1:C:525:GLN:HG2	2.43	0.47
1:D:436:CYS:O	1:D:439:LYS:HB2	2.14	0.47
1:A:160:TYR:O	1:A:163:VAL:HB	2.14	0.47
1:B:484:ARG:CB	1:B:485:PRO:CD	2.89	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HB3	1:A:373:PHE:CZ	2.50	0.47
1:A:531:LEU:HD21	1:A:546:VAL:HG11	1.95	0.47
1:C:266:HIS:O	1:C:269:THR:OG1	2.23	0.47
1:C:407:ILE:HG13	1:C:426:SER:CB	2.45	0.47
1:D:562:ASP:HB2	5:D:816:HOH:O	2.14	0.47
1:C:50:ALA:C	1:C:52:THR:N	2.66	0.47
1:A:310:GLU:HA	1:A:366:HIS:NE2	2.29	0.47
1:A:43:VAL:O	1:A:43:VAL:HG12	2.14	0.47
1:B:515:LEU:O	1:B:520:LYS:HE3	2.15	0.47
1:B:5:SER:CB	1:B:62:CYS:O	2.63	0.47
1:C:261:LYS:HD3	5:C:715:HOH:O	2.14	0.47
1:D:510:ALA:C	1:D:512:ILE:N	2.66	0.47
1:B:261:LYS:HB3	5:B:762:HOH:O	2.15	0.47
1:B:542:GLN:O	1:B:546:VAL:HG23	2.14	0.47
1:C:421:THR:O	1:C:425:ILE:HG12	2.15	0.47
1:D:207:GLU:OE1	1:D:242:LYS:CE	2.63	0.47
1:B:140:GLU:OE1	1:B:144:ARG:NH1	2.46	0.47
1:C:182:GLU:HA	1:C:182:GLU:OE1	2.15	0.47
1:C:95:GLU:OE2	1:C:96:PRO:HA	2.15	0.47
1:C:150:ALA:HB2	1:C:249:LEU:HD22	1.95	0.46
1:C:544:LYS:HE2	1:C:548:GLU:OE2	2.15	0.46
1:D:419:THR:O	1:D:423:VAL:HG23	2.15	0.46
1:A:213:TRP:HB2	3:A:602:PRO:O	2.16	0.46
1:B:348:LEU:O	1:B:352:TYR:N	2.45	0.46
1:C:110:PRO:HG3	1:C:144:ARG:HA	1.97	0.46
1:C:415:PRO:HD2	1:C:416:GLN:OE1	2.14	0.46
1:D:61:GLY:O	1:D:64:LYS:HG3	2.15	0.46
1:A:236:ASP:HB2	1:A:259:LEU:HD13	1.96	0.46
1:A:311:ASP:HB3	1:A:314:VAL:HG23	1.97	0.46
1:B:408:VAL:O	1:B:412:ARG:HG3	2.15	0.46
1:D:470:GLU:HA	1:D:473:THR:CG2	2.45	0.46
1:A:359:CYS:O	1:A:361:ALA:N	2.49	0.46
1:A:415:PRO:HG2	1:A:496:TYR:CG	2.51	0.46
1:B:490:LEU:HA	5:B:738:HOH:O	2.15	0.46
1:D:419:THR:HG21	1:D:526:THR:HG23	1.96	0.46
1:B:54:VAL:HB	5:B:760:HOH:O	2.15	0.46
1:B:134:TRP:CG	3:B:602:PRO:HD3	2.50	0.46
1:C:395:GLU:OE1	1:C:395:GLU:HA	2.16	0.46
1:C:419:THR:HB	1:C:420:PRO:CD	2.45	0.46
1:C:507:THR:HG23	1:C:509:HIS:CE1	2.50	0.46
1:D:364:ASP:HB3	1:D:367:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:O	1:A:48:GLU:HG2	2.14	0.46
1:A:452:LEU:CD1	1:A:484:ARG:HD2	2.45	0.46
1:B:301:LEU:HB3	1:B:336:ARG:HH11	1.80	0.46
1:C:187:LYS:O	1:C:190:ALA:HB3	2.16	0.46
1:C:236:ASP:CB	1:C:259:LEU:HD13	2.46	0.46
1:C:416:GLN:HB2	1:C:469:SER:HB2	1.97	0.46
1:C:519:GLU:N	1:C:519:GLU:OE1	2.48	0.46
1:D:433:GLY:O	1:D:437:CYS:HB2	2.16	0.46
1:A:233:ILE:HG23	1:A:259:LEU:HD11	1.98	0.46
1:A:304:LEU:HD11	1:A:333:TYR:HA	1.98	0.46
1:A:386:LEU:CD2	1:A:484:ARG:HH21	2.29	0.46
1:C:441:GLU:HA	1:C:444:ARG:NH1	2.30	0.46
1:A:275:LYS:HD2	1:A:275:LYS:HA	1.68	0.46
1:A:392:GLU:O	1:A:393:LEU:C	2.52	0.46
1:A:470:GLU:CD	1:A:470:GLU:H	2.19	0.46
1:B:386:LEU:HD21	1:B:484:ARG:HH12	1.81	0.46
1:A:478:GLU:O	1:A:479:SER:C	2.53	0.46
1:C:388:LYS:O	1:C:392:GLU:HG3	2.16	0.46
1:C:43:VAL:O	1:C:47:THR:OG1	2.27	0.46
1:D:131:LYS:HE3	3:D:602:PRO:HB2	1.96	0.46
1:D:141:VAL:O	1:D:145:HIS:HD2	1.99	0.46
1:D:419:THR:HG23	1:D:529:VAL:HG11	1.97	0.46
1:D:467:PRO:HB2	3:D:605:PRO:CD	2.46	0.46
1:A:16:GLU:HB3	3:A:603:PRO:HG3	1.98	0.46
1:B:71:GLY:C	1:B:73:GLU:H	2.18	0.46
1:D:539:THR:HG23	1:D:542:GLN:OE1	2.16	0.46
1:A:310:GLU:O	1:A:311:ASP:C	2.53	0.45
1:A:347:ARG:HH21	1:A:485:PRO:CD	2.29	0.45
1:A:68:THR:HA	1:A:98:ARG:HH12	1.81	0.45
1:D:550:PHE:O	1:D:554:VAL:HG23	2.17	0.45
1:A:331:TYR:OH	1:A:335:ARG:NH1	2.50	0.45
1:B:324:VAL:O	1:B:325:PHE:C	2.54	0.45
1:B:439:LYS:O	1:B:440:PRO:C	2.54	0.45
1:C:160:TYR:O	1:C:164:PHE:HD2	1.99	0.45
1:A:384:GLN:O	1:A:388:LYS:HD2	2.16	0.45
1:A:553:PHE:CZ	1:A:567:PHE:CD1	3.04	0.45
1:A:9:HIS:CD2	1:A:9:HIS:C	2.88	0.45
1:B:81:ARG:HG3	1:B:88:ALA:HB2	1.97	0.45
1:A:415:PRO:HD2	1:A:416:GLN:HE22	1.77	0.45
1:A:387:ILE:HG13	1:A:448:THR:HG21	1.98	0.45
1:A:515:LEU:HB3	1:A:519:GLU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ASN:ND2	5:B:709:HOH:O	2.44	0.45
1:D:148:PHE:CD1	1:D:149:TYR:O	2.69	0.45
1:C:89:ASP:C	1:C:92:GLU:HB3	2.36	0.45
1:D:59:HIS:ND1	1:D:60:ALA:N	2.64	0.45
1:A:264:CYS:O	1:A:267:GLN:CG	2.61	0.45
1:B:419:THR:HB	1:B:420:PRO:HD3	1.99	0.45
1:C:544:LYS:HB2	5:C:783:HOH:O	2.17	0.45
1:D:470:GLU:O	1:D:473:THR:HG22	2.17	0.45
1:D:545:THR:O	1:D:548:GLU:N	2.48	0.45
1:A:407:ILE:O	1:A:411:THR:OG1	2.18	0.45
1:B:163:VAL:O	1:B:167:CYS:HB2	2.17	0.45
1:C:152:GLU:OE1	1:C:287:HIS:ND1	2.38	0.45
1:C:189:LEU:O	1:C:190:ALA:C	2.55	0.45
1:C:473:THR:HG23	5:C:811:HOH:O	2.16	0.45
1:C:542:GLN:NE2	1:C:582:LEU:HA	2.32	0.45
1:B:347:ARG:HG3	1:B:481:VAL:HG12	1.99	0.45
1:C:419:THR:HG23	1:C:529:VAL:CG1	2.47	0.45
1:C:506:PHE:CZ	1:C:550:PHE:CE1	3.05	0.45
1:C:83:THR:O	1:C:83:THR:HG22	2.17	0.45
1:D:464:GLU:HB2	5:D:739:HOH:O	2.17	0.45
1:C:101:CYS:O	1:C:104:LYS:HB2	2.16	0.45
1:A:132:LYS:O	1:A:136:LYS:HB2	2.15	0.45
1:A:137:TYR:O	1:A:141:VAL:HG23	2.17	0.45
1:A:463:HIS:CD2	1:A:472:VAL:CG1	2.99	0.45
1:A:347:ARG:HH22	1:A:484:ARG:HH12	1.66	0.45
1:B:197:LEU:O	1:B:198:ARG:C	2.54	0.45
1:C:6:GLU:HG3	1:C:66:LEU:HD11	1.97	0.45
1:D:16:GLU:O	1:D:20:GLN:HG3	2.17	0.45
1:D:151:PRO:HG2	1:D:256:ARG:HD3	1.98	0.45
1:B:257:ALA:O	1:B:260:ALA:HB3	2.17	0.44
1:D:131:LYS:CE	3:D:602:PRO:CB	2.94	0.44
1:D:178:LEU:HB2	1:D:179:PRO:HD3	1.99	0.44
1:A:512:ILE:O	1:A:520:LYS:HE3	2.17	0.44
1:A:9:HIS:HE1	5:A:783:HOH:O	1.99	0.44
1:B:274:LEU:HD23	1:B:274:LEU:HA	1.69	0.44
1:C:389:LYS:HA	1:C:392:GLU:OE2	2.16	0.44
1:D:9:HIS:NE2	5:D:703:HOH:O	2.36	0.44
1:A:347:ARG:HH21	1:A:485:PRO:HD3	1.82	0.44
1:B:416:GLN:H	1:B:416:GLN:CD	2.21	0.44
1:C:281:PRO:O	1:C:285:LYS:N	2.50	0.44
1:C:301:LEU:HB3	1:C:336:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:LEU:HD22	1:C:570:GLU:CG	2.34	0.44
1:D:268:ASP:N	1:D:268:ASP:OD1	2.37	0.44
1:B:66:LEU:HD23	1:B:69:LEU:HD12	2.00	0.44
1:B:73:GLU:C	1:B:75:CYS:N	2.65	0.44
1:B:236:ASP:O	1:B:240:VAL:HG23	2.18	0.44
1:C:390:ASN:ND2	3:C:604:PRO:OXT	2.51	0.44
1:D:501:PHE:O	1:D:504:GLU:HB2	2.18	0.44
1:D:158:ASN:OD1	3:D:602:PRO:HD3	2.17	0.44
1:A:243:GLU:OE2	1:A:251:GLU:HB3	2.18	0.44
1:A:44:LYS:HA	1:A:47:THR:HB	1.99	0.44
1:B:445:MET:O	1:B:446:PRO:C	2.54	0.44
1:B:52:THR:C	1:B:54:VAL:N	2.71	0.44
1:D:233:ILE:HG23	1:D:259:LEU:HD11	1.98	0.44
1:B:195:GLN:O	1:B:196:ARG:C	2.56	0.44
1:B:396:LYS:HB2	1:B:396:LYS:HE3	1.71	0.44
1:A:4:LYS:HG2	1:A:57:GLU:OE2	2.16	0.44
1:B:237:LEU:CD1	1:B:241:HIS:CE1	3.01	0.44
1:C:313:GLU:O	1:C:314:VAL:C	2.55	0.44
1:D:229:ASP:O	1:D:230:VAL:C	2.56	0.44
1:D:382:GLU:CB	1:D:383:PRO:CD	2.87	0.44
1:A:116:LYS:HA	1:A:117:PRO:HD2	1.89	0.44
1:A:217:ARG:CG	1:A:218:LEU:N	2.77	0.44
1:A:221:LYS:C	1:A:222:PHE:HD1	2.21	0.44
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.83	0.44
1:C:396:LYS:HB3	1:C:397:HIS:CD2	2.53	0.44
1:C:512:ILE:HA	1:C:515:LEU:HD12	1.99	0.44
1:D:340:TYR:HA	1:D:445:MET:CE	2.48	0.44
1:B:139:TYR:CE1	1:B:143:ARG:HD2	2.53	0.43
1:B:257:ALA:HA	1:B:260:ALA:HB3	2.00	0.43
1:B:493:ASP:OD1	1:B:495:THR:HB	2.17	0.43
1:B:539:THR:CG2	1:B:541:GLU:HG2	2.48	0.43
1:D:164:PHE:CE1	1:D:177:LEU:HD21	2.54	0.43
1:A:333:TYR:HE1	1:A:340:TYR:HE2	1.66	0.43
1:C:223:PRO:HB3	1:C:335:ARG:HB2	2.00	0.43
1:C:539:THR:HB	1:C:542:GLN:H	1.82	0.43
1:A:31:LEU:HB2	1:A:39:HIS:NE2	2.33	0.43
1:A:43:VAL:CG1	1:A:43:VAL:O	2.66	0.43
1:A:386:LEU:HD21	1:A:484:ARG:HH21	1.83	0.43
1:B:333:TYR:HD2	1:B:333:TYR:O	2.02	0.43
1:B:380:VAL:O	1:B:384:GLN:HG3	2.17	0.43
1:B:486:CYS:O	1:B:489:ASP:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LEU:CD2	1:B:516:PRO:HD2	2.46	0.43
1:B:51:LYS:HE2	1:B:51:LYS:HB2	1.74	0.43
1:C:484:ARG:O	1:C:488:SER:HB2	2.18	0.43
1:D:217:ARG:NH1	5:D:718:HOH:O	2.51	0.43
1:D:411:THR:HA	1:D:422:LEU:HD22	1.99	0.43
1:D:95:GLU:OE2	1:D:96:PRO:HA	2.19	0.43
1:A:140:GLU:OE1	1:A:140:GLU:HA	2.19	0.43
1:A:452:LEU:HD13	1:A:484:ARG:HD2	2.00	0.43
1:A:6:GLU:OE1	1:A:6:GLU:HA	2.19	0.43
1:D:61:GLY:HA2	1:D:64:LYS:HE3	2.01	0.43
1:A:250:LEU:O	1:A:254:ASP:HB2	2.18	0.43
1:A:275:LYS:HD2	1:A:278:CYS:HB2	2.01	0.43
1:C:161:ASN:ND2	3:C:603:PRO:HA	2.33	0.43
1:C:408:VAL:HA	1:C:532:LEU:CD1	2.48	0.43
1:C:412:ARG:HB3	1:C:492:LEU:HD13	2.01	0.43
1:C:550:PHE:CD1	1:C:574:LEU:HD21	2.53	0.43
1:A:508:PHE:N	1:A:508:PHE:CD1	2.84	0.43
1:B:90:CYS:HB3	1:B:101:CYS:HB3	1.91	0.43
1:C:318:TYR:CZ	1:C:322:LYS:HE2	2.53	0.43
1:D:379:LEU:O	1:D:382:GLU:HG3	2.19	0.43
1:D:81:ARG:CG	1:D:88:ALA:HB3	2.43	0.43
1:B:433:GLY:HA2	1:B:437:CYS:SG	2.58	0.43
1:B:47:THR:O	1:B:50:ALA:HB3	2.19	0.43
1:C:109:SER:HA	5:C:766:HOH:O	2.17	0.43
1:D:407:ILE:HG13	1:D:426:SER:CB	2.48	0.43
1:B:273:LYS:NZ	1:B:294:LYS:O	2.52	0.43
1:B:366:HIS:O	1:B:370:ALA:HB2	2.19	0.43
1:B:396:LYS:HG3	1:B:397:HIS:ND1	2.34	0.43
1:B:48:GLU:OE1	1:B:51:LYS:NZ	2.52	0.43
1:B:93:LYS:HG2	1:B:93:LYS:H	1.51	0.43
1:C:417:VAL:HA	5:C:765:HOH:O	2.18	0.43
1:A:8:ALA:HB2	1:A:53:CYS:HB2	2.01	0.42
1:C:313:GLU:HG3	1:C:313:GLU:H	1.62	0.42
1:D:341:ALA:H	1:D:445:MET:CE	2.32	0.42
1:A:406:LEU:HD13	1:A:429:LEU:CB	2.49	0.42
1:B:21:GLY:O	1:B:24:LEU:HB3	2.19	0.42
1:A:345:LEU:O	1:A:346:LEU:C	2.58	0.42
1:B:32:GLN:HA	1:B:143:ARG:HB2	2.01	0.42
1:B:29:GLN:NE2	1:B:146:PRO:HA	2.33	0.42
1:C:160:TYR:CE1	1:C:164:PHE:HE2	2.37	0.42
1:C:299:GLU:HG2	1:C:300:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:VAL:HG13	1:C:335:ARG:O	2.18	0.42
1:C:36:PHE:O	1:C:40:VAL:HG23	2.19	0.42
1:C:417:VAL:HG12	1:C:422:LEU:HG	2.01	0.42
1:A:226:ASP:HB2	1:A:229:ASP:HB2	2.02	0.42
1:B:382:GLU:HB2	1:B:383:PRO:CD	2.50	0.42
1:B:73:GLU:O	1:B:74:LEU:C	2.56	0.42
1:C:470:GLU:HB3	5:C:752:HOH:O	2.19	0.42
1:D:246:HIS:O	1:D:246:HIS:CG	2.72	0.42
1:D:318:TYR:OH	1:D:357:GLU:OE1	2.31	0.42
1:D:5:SER:HB2	1:D:62:CYS:O	2.19	0.42
1:B:496:TYR:HE2	1:B:536:PRO:HG3	1.84	0.42
1:C:39:HIS:CE1	1:C:139:TYR:HE1	2.37	0.42
1:C:566:CYS:C	1:C:568:LEU:N	2.72	0.42
1:C:80:LEU:HD11	1:C:87:MET:SD	2.59	0.42
1:D:61:GLY:HA2	1:D:64:LYS:CE	2.49	0.42
1:A:207:GLU:HG3	5:A:785:HOH:O	2.18	0.42
1:C:165:GLN:OE1	1:C:165:GLN:HA	2.20	0.42
1:C:419:THR:HG22	1:C:526:THR:HG23	2.02	0.42
1:A:223:PRO:HA	1:A:335:ARG:HB2	2.02	0.42
1:A:36:PHE:O	1:A:40:VAL:HG23	2.20	0.42
1:A:419:THR:HG23	1:A:529:VAL:CG1	2.49	0.42
1:A:539:THR:HB	1:A:542:GLN:HB2	2.01	0.42
1:B:110:PRO:HG3	1:B:144:ARG:HA	2.01	0.42
1:B:29:GLN:NE2	1:B:146:PRO:C	2.73	0.42
1:D:194:ARG:HD2	1:D:198:ARG:NH2	2.35	0.42
1:D:563:LYS:HB2	5:D:772:HOH:O	2.20	0.42
1:A:299:GLU:HG2	1:A:299:GLU:H	1.58	0.42
1:B:535:LYS:CE	1:B:583:ALA:HA	2.49	0.42
1:A:59:HIS:CD2	1:A:60:ALA:H	2.38	0.42
1:B:341:ALA:HB1	1:B:449:GLU:HB2	2.01	0.42
1:C:251:GLU:H	1:C:251:GLU:CD	2.20	0.42
1:D:242:LYS:HB2	1:D:242:LYS:HE3	1.83	0.42
1:D:502:ASP:C	1:D:504:GLU:H	2.23	0.42
1:B:341:ALA:HB3	1:B:344:VAL:HG23	2.02	0.42
1:C:164:PHE:CE1	1:C:177:LEU:HD22	2.55	0.42
1:D:112:LEU:HB3	1:D:113:PRO:HD2	2.02	0.42
1:D:246:HIS:O	1:D:246:HIS:ND1	2.53	0.42
1:D:538:ALA:HA	5:D:784:HOH:O	2.19	0.42
1:D:550:PHE:HE2	1:D:574:LEU:HD21	1.81	0.42
1:D:77:VAL:HG12	1:D:77:VAL:O	2.20	0.42
1:B:391:CYS:O	1:B:395:GLU:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:CYS:HA	1:D:439:LYS:HD2	2.01	0.41
1:A:225:ALA:HB2	1:A:270:LEU:HA	2.02	0.41
1:A:35:PRO:O	1:A:38:GLU:HB2	2.20	0.41
1:B:387:ILE:N	1:B:387:ILE:HD13	2.34	0.41
1:C:6:GLU:HA	1:C:6:GLU:OE1	2.20	0.41
1:D:129:ASP:O	1:D:130:GLU:C	2.58	0.41
1:A:167:CYS:O	1:A:168:CYS:C	2.58	0.41
1:C:196:ARG:HD2	1:C:196:ARG:HA	1.74	0.41
1:C:391:CYS:O	1:C:395:GLU:HG2	2.20	0.41
1:D:299:GLU:HA	5:D:728:HOH:O	2.19	0.41
1:D:565:GLY:O	1:D:569:LEU:HD12	2.20	0.41
1:A:254:ASP:O	1:A:257:ALA:HB3	2.19	0.41
1:A:371:THR:O	1:A:371:THR:HG22	2.20	0.41
1:B:237:LEU:HD11	1:B:241:HIS:NE2	2.36	0.41
1:B:303:PRO:HD3	3:B:603:PRO:HA	2.01	0.41
1:C:499:LYS:HA	1:C:499:LYS:HD2	1.86	0.41
1:D:116:LYS:HA	1:D:117:PRO:HD2	1.83	0.41
1:D:229:ASP:O	1:D:233:ILE:HG13	2.21	0.41
1:D:103:LEU:HD11	1:D:246:HIS:O	2.20	0.41
1:D:36:PHE:O	1:D:40:VAL:HG23	2.21	0.41
1:A:304:LEU:HD23	1:A:308:PHE:CD2	2.55	0.41
1:A:438:ALA:HB3	5:A:751:HOH:O	2.21	0.41
1:B:301:LEU:HD13	1:B:336:ARG:NH1	2.36	0.41
1:C:429:LEU:HD23	1:C:429:LEU:HA	1.68	0.41
1:C:544:LYS:HG2	5:C:733:HOH:O	2.20	0.41
1:D:273:LYS:C	1:D:292:ILE:HD11	2.40	0.41
1:D:440:PRO:O	1:D:444:ARG:HG3	2.20	0.41
1:D:512:ILE:O	1:D:520:LYS:HE3	2.20	0.41
1:A:347:ARG:HH21	1:A:485:PRO:CG	2.34	0.41
1:C:22:LEU:O	1:C:26:ALA:N	2.45	0.41
1:D:374:ASP:N	1:D:374:ASP:OD1	2.53	0.41
1:D:403:GLN:HG2	1:D:427:ARG:HA	2.02	0.41
1:D:6:GLU:HG3	1:D:66:LEU:HD11	2.02	0.41
1:A:21:GLY:HA3	1:A:154:LEU:HD21	2.03	0.41
1:A:553:PHE:CZ	1:A:567:PHE:HD1	2.39	0.41
1:B:550:PHE:HD2	1:B:574:LEU:HD11	1.86	0.41
1:C:340:TYR:CZ	1:C:380:VAL:HG21	2.55	0.41
1:A:337:HIS:C	1:A:339:GLU:H	2.22	0.41
1:B:25:ILE:O	1:B:26:ALA:C	2.59	0.41
1:C:412:ARG:CB	1:C:492:LEU:HD13	2.50	0.41
1:A:16:GLU:CG	3:A:603:PRO:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ALA:O	1:B:417:VAL:HG23	2.20	0.41
1:C:218:LEU:HA	1:C:218:LEU:HD23	1.67	0.41
1:C:505:SER:HB2	1:C:530:GLU:HG3	2.01	0.41
1:C:390:ASN:CB	3:C:604:PRO:HB3	2.50	0.41
1:D:393:LEU:HD12	1:D:393:LEU:HA	1.86	0.41
1:D:404:ASN:OD1	1:D:525:GLN:HG2	2.21	0.41
1:A:334:SER:C	1:A:336:ARG:N	2.74	0.41
1:A:492:LEU:HD12	1:A:492:LEU:N	2.34	0.41
1:B:6:GLU:OE2	1:B:10:ARG:NE	2.54	0.41
1:C:130:GLU:HG2	3:C:603:PRO:HB2	2.02	0.41
1:D:17:GLU:OE1	3:D:602:PRO:HB2	2.20	0.41
1:A:535:LYS:HA	1:A:536:PRO:HD2	1.79	0.41
1:B:232:LYS:HD3	1:B:236:ASP:OD1	2.21	0.41
1:C:129:ASP:HB3	1:C:132:LYS:HB3	2.03	0.41
1:C:429:LEU:HD23	1:C:455:ILE:HD13	2.03	0.41
1:D:563:LYS:H	1:D:563:LYS:HG3	1.73	0.41
1:D:71:GLY:HA3	1:D:98:ARG:HH11	1.84	0.41
1:A:214:SER:CB	1:A:234:VAL:HG22	2.51	0.40
1:B:160:TYR:O	1:B:164:PHE:HD2	2.04	0.40
1:B:512:ILE:HD13	1:B:554:VAL:HG11	2.02	0.40
1:D:237:LEU:HA	1:D:237:LEU:HD12	1.82	0.40
1:D:342:VAL:HG21	3:D:603:PRO:HD2	2.03	0.40
1:A:332:GLU:O	1:A:336:ARG:HD2	2.21	0.40
1:A:334:SER:OG	1:A:345:LEU:HD13	2.21	0.40
1:A:83:THR:HB	1:A:84:TYR:CE2	2.57	0.40
1:B:171:GLU:CD	1:B:171:GLU:H	2.21	0.40
1:B:436:CYS:O	1:B:439:LYS:HB2	2.21	0.40
1:B:9:HIS:CE1	1:B:13:ASP:OD2	2.74	0.40
1:C:535:LYS:HG3	1:C:582:LEU:HD13	2.04	0.40
1:C:81:ARG:HD3	1:C:88:ALA:CB	2.51	0.40
1:A:258:ASP:O	1:A:259:LEU:C	2.57	0.40
1:A:353:GLU:HG2	5:A:704:HOH:O	2.22	0.40
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.36	0.40
1:C:271:SER:HB3	1:C:274:LEU:HD12	2.03	0.40
1:C:375:LYS:O	1:C:376:LEU:C	2.58	0.40
1:D:13:ASP:OD1	1:D:254:ASP:OD2	2.39	0.40
1:A:436:CYS:O	1:A:438:ALA:N	2.54	0.40
1:B:52:THR:O	1:B:55:ALA:N	2.55	0.40
1:B:33:GLN:HB2	1:B:84:TYR:CZ	2.56	0.40
1:C:232:LYS:O	1:C:232:LYS:HD3	2.21	0.40
1:D:196:ARG:HH12	1:D:200:ALA:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:NZ	1:B:116:LYS:HG2	2.37	0.40
1:A:289:ILE:O	1:A:292:ILE:HG22	2.21	0.40
1:A:414:ALA:HB1	1:A:417:VAL:HG23	2.04	0.40
1:A:456:LEU:HA	1:A:456:LEU:HD23	1.82	0.40
1:B:224:LYS:HE3	1:B:268:ASP:O	2.21	0.40
1:B:257:ALA:O	1:B:261:LYS:N	2.38	0.40
1:B:416:GLN:NE2	1:B:496:TYR:HB2	2.37	0.40
1:B:533:LYS:O	1:B:536:PRO:HD3	2.21	0.40
1:C:223:PRO:CB	1:C:335:ARG:HB2	2.51	0.40
1:C:402:PHE:O	1:C:405:ALA:HB3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:NZ	1:D:313:GLU:OE2[1_545]	2.05	0.15
1:C:312:LYS:NZ	1:D:361:ALA:O[1_546]	2.15	0.05

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	579/583 (99%)	518 (90%)	58 (10%)	3 (0%)	29	48
1	B	579/583 (99%)	523 (90%)	54 (9%)	2 (0%)	41	61
1	C	579/583 (99%)	515 (89%)	62 (11%)	2 (0%)	41	61
1	D	580/583 (100%)	517 (89%)	60 (10%)	3 (0%)	29	48
All	All	2317/2332 (99%)	2073 (90%)	234 (10%)	10 (0%)	34	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	499	LYS
1	A	269	THR
1	B	441	GLU
1	D	79	THR
1	A	360	CYS
1	D	92	GLU
1	D	500	PRO
1	C	382	GLU
1	A	485	PRO
1	C	468	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	515/517 (100%)	477 (93%)	38 (7%)	13	27
1	B	515/517 (100%)	487 (95%)	28 (5%)	22	42
1	C	515/517 (100%)	482 (94%)	33 (6%)	17	33
1	D	516/517 (100%)	483 (94%)	33 (6%)	17	33
All	All	2061/2068 (100%)	1929 (94%)	132 (6%)	17	33

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	12	ASN
1	A	68	THR
1	A	86	ASP
1	A	91	CYS
1	A	104	LYS
1	A	131	LYS
1	A	149	TYR
1	A	153	LEU
1	A	217	ARG
1	A	221	LYS
1	A	224	LYS

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Mol	Chain	Res	Type
1	A	268	ASP
1	A	275	LYS
1	A	299	GLU
1	A	304	LEU
1	A	312	LYS
1	A	328	SER
1	A	347	ARG
1	A	358	ASP
1	A	362	LYS
1	A	369	TYR
1	A	386	LEU
1	A	392	GLU
1	A	431	LYS
1	A	439	LYS
1	A	466	THR
1	A	479	SER
1	A	483	ARG
1	A	491	THR
1	A	493	ASP
1	A	495	THR
1	A	501	PHE
1	A	507	THR
1	A	523	LYS
1	A	541	GLU
1	A	545	THR
1	A	582	LEU
1	B	3	HIS
1	B	6	GLU
1	B	7	ILE
1	B	38	GLU
1	B	49	PHE
1	B	80	LEU
1	B	91	CYS
1	B	118	GLU
1	B	161	ASN
1	B	202	ILE
1	B	213	TRP
1	B	229	ASP
1	B	268	ASP
1	B	272	SER
1	B	275	LYS
1	B	311	ASP

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Mol	Chain	Res	Type
1	B	312	LYS
1	B	313	GLU
1	B	319	GLN
1	B	331	TYR
1	B	333	TYR
1	B	343	SER
1	B	356	LEU
1	B	369	TYR
1	B	450	ASP
1	B	511	ASP
1	B	517	ASP
1	B	544	LYS
1	C	34	CYS
1	C	38	GLU
1	C	47	THR
1	C	51	LYS
1	C	52	THR
1	C	54	VAL
1	C	72	ASP
1	C	105	HIS
1	C	116	LYS
1	C	129	ASP
1	C	131	LYS
1	C	149	TYR
1	C	161	ASN
1	C	177	LEU
1	C	213	TRP
1	C	221	LYS
1	C	235	THR
1	C	268	ASP
1	C	312	LYS
1	C	336	ARG
1	C	350	LYS
1	C	356	LEU
1	C	366	HIS
1	C	461	VAL
1	C	474	LYS
1	C	484	ARG
1	C	495	THR
1	C	499	LYS
1	C	501	PHE
1	C	506	PHE

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Mol	Chain	Res	Type
1	C	519	GLU
1	C	537	LYS
1	C	556	LYS
1	D	13	ASP
1	D	17	GLU
1	D	44	LYS
1	D	47	THR
1	D	77	VAL
1	D	104	LYS
1	D	130	GLU
1	D	131	LYS
1	D	149	TYR
1	D	171	GLU
1	D	204	LYS
1	D	227	PHE
1	D	239	LYS
1	D	268	ASP
1	D	271	SER
1	D	292	ILE
1	D	293	ASP
1	D	300	ASN
1	D	307	ASP
1	D	312	LYS
1	D	314	VAL
1	D	374	ASP
1	D	377	LYS
1	D	386	LEU
1	D	388	LYS
1	D	480	LEU
1	D	491	THR
1	D	501	PHE
1	D	507	THR
1	D	518	THR
1	D	563	LYS
1	D	564	GLU
1	D	582	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	HIS
1	A	317	ASN

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Mol	Chain	Res	Type
1	A	463	HIS
1	B	29	GLN
1	B	33	GLN
1	B	67	HIS
1	B	463	HIS
1	C	300	ASN
1	C	397	HIS
1	C	509	HIS
1	D	20	GLN
1	D	145	HIS
1	D	463	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

16 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	PGE	A	601	-	9,9,9	0.60	0	8,8,8	0.29	0
4	PEG	C	602	-	6,6,6	0.47	0	5,5,5	0.52	0
2	PGE	C	601	-	9,9,9	0.59	0	8,8,8	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PGE	B	601	-	9,9,9	0.56	0	8,8,8	0.78	0
4	PEG	D	601	-	6,6,6	0.45	0	5,5,5	0.34	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	PGE	A	601	-	-	4/7/7/7	-
4	PEG	C	602	-	-	3/4/4/4	-
2	PGE	C	601	-	-	3/7/7/7	-
2	PGE	B	601	-	-	5/7/7/7	-
4	PEG	D	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	601	PEG	O2-C3-C4-O4
2	A	601	PGE	O1-C1-C2-O2
2	C	601	PGE	O3-C5-C6-O4
2	A	601	PGE	O3-C5-C6-O4
4	C	602	PEG	O1-C1-C2-O2
2	B	601	PGE	O2-C3-C4-O3
2	B	601	PGE	O3-C5-C6-O4
2	C	601	PGE	C6-C5-O3-C4
4	C	602	PEG	C4-C3-O2-C2
2	A	601	PGE	C3-C4-O3-C5
2	C	601	PGE	C3-C4-O3-C5
2	B	601	PGE	C4-C3-O2-C2
4	C	602	PEG	O2-C3-C4-O4
2	B	601	PGE	O1-C1-C2-O2
2	A	601	PGE	O2-C3-C4-O3
2	B	601	PGE	C3-C4-O3-C5
4	D	601	PEG	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PGE	1	0
4	C	602	PEG	1	0
2	B	601	PGE	1	0
4	D	601	PEG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	581/583 (99%)	-0.16	16 (2%)	53	56	33, 62, 96, 118	0
1	B	581/583 (99%)	-0.01	29 (4%)	28	30	33, 60, 104, 138	0
1	C	581/583 (99%)	0.02	31 (5%)	26	28	36, 62, 106, 154	0
1	D	581/583 (99%)	-0.19	16 (2%)	53	56	32, 60, 97, 133	0
All	All	2324/2332 (99%)	-0.09	92 (3%)	38	41	32, 61, 102, 154	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	PHE	5.3
1	C	501	PHE	5.1
1	C	500	PRO	4.8
1	B	89	ASP	4.7
1	D	81	ARG	4.4
1	B	583	ALA	4.2
1	D	3	HIS	4.2
1	D	500	PRO	4.2
1	D	582	LEU	4.2
1	B	5	SER	4.0
1	B	93	LYS	3.7
1	C	83	THR	3.7
1	A	503	GLY	3.7
1	C	497	VAL	3.6
1	C	386	LEU	3.6
1	B	500	PRO	3.5
1	D	501	PHE	3.5
1	A	89	ASP	3.5
1	C	85	GLY	3.5
1	C	503	GLY	3.4
1	C	46	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	84	TYR	3.3
1	B	582	LEU	3.3
1	A	31	LEU	3.2
1	B	502	ASP	3.2
1	C	75	CYS	3.1
1	C	574	LEU	3.0
1	A	575	VAL	3.0
1	A	505	SER	3.0
1	B	83	THR	3.0
1	B	581	ALA	3.0
1	C	84	TYR	2.9
1	B	27	PHE	2.8
1	C	91	CYS	2.8
1	B	76	LYS	2.8
1	D	75	CYS	2.8
1	B	501	PHE	2.8
1	D	503	GLY	2.7
1	A	582	LEU	2.7
1	C	575	VAL	2.7
1	B	367	ALA	2.7
1	B	575	VAL	2.7
1	B	84	TYR	2.7
1	A	569	LEU	2.7
1	A	83	THR	2.6
1	D	583	ALA	2.6
1	C	583	ALA	2.6
1	A	500	PRO	2.6
1	C	534	HIS	2.6
1	C	30	TYR	2.6
1	A	501	PHE	2.6
1	C	504	GLU	2.5
1	B	580	ALA	2.5
1	D	83	THR	2.5
1	C	80	LEU	2.5
1	D	87	MET	2.5
1	B	82	GLU	2.5
1	C	582	LEU	2.4
1	A	30	TYR	2.4
1	B	90	CYS	2.4
1	B	7	ILE	2.4
1	B	78	ALA	2.4
1	A	82	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	3	HIS	2.4
1	D	531	LEU	2.4
1	C	5	SER	2.4
1	B	574	LEU	2.3
1	C	31	LEU	2.3
1	C	492	LEU	2.3
1	D	86	ASP	2.3
1	B	546	VAL	2.3
1	C	82	GLU	2.3
1	D	80	LEU	2.3
1	B	505	SER	2.2
1	A	78	ALA	2.2
1	B	55	ALA	2.1
1	C	88	ALA	2.1
1	B	506	PHE	2.1
1	C	506	PHE	2.1
1	D	11	PHE	2.1
1	B	88	ALA	2.1
1	B	503	GLY	2.1
1	B	81	ARG	2.1
1	A	93	LYS	2.1
1	A	502	ASP	2.1
1	C	74	LEU	2.1
1	B	270	LEU	2.0
1	C	27	PHE	2.0
1	D	492	LEU	2.0
1	C	69	LEU	2.0
1	D	79	THR	2.0
1	C	86	ASP	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. 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	B-factors(Å^2)	Q<0.9
3	PRO	B	603	8/8	0.79	0.17	80,86,91,92	0
3	PRO	D	603	8/8	0.85	0.29	74,86,104,105	0
3	PRO	B	602	8/8	0.87	0.25	75,88,94,97	0
3	PRO	D	604	8/8	0.88	0.14	66,77,83,86	0
3	PRO	A	603	8/8	0.89	0.14	81,82,90,92	0
3	PRO	C	604	8/8	0.90	0.17	68,74,81,90	0
3	PRO	C	603	8/8	0.92	0.21	74,84,86,90	0
3	PRO	D	605	8/8	0.92	0.13	80,83,100,100	0
3	PRO	A	602	8/8	0.93	0.21	78,84,88,92	0
3	PRO	C	605	8/8	0.93	0.28	78,88,91,91	0
2	PGE	C	601	10/10	0.94	0.14	52,61,68,75	0
4	PEG	D	601	7/7	0.94	0.15	52,53,62,63	0
3	PRO	D	602	8/8	0.95	0.16	61,70,89,100	0
4	PEG	C	602	7/7	0.95	0.20	55,66,77,83	0
2	PGE	A	601	10/10	0.96	0.20	47,71,85,97	0
2	PGE	B	601	10/10	0.97	0.16	45,55,86,87	0

6.5 Other polymers (i)

There are no such residues in this entry.