



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:21 PM GMT

PDB ID : 4C7R
Title : Inward facing conformation of the trimeric betaine transporter BetP in complex with lipids
Authors : Koshy, C.; Yildiz, O.; Ziegler, C.
Deposited on : 2013-09-24
Resolution : 2.70 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

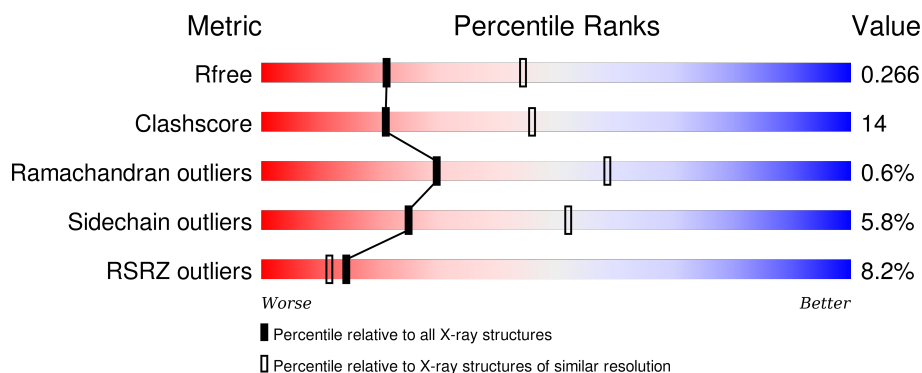
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	566	<div> <div>6%</div> <div>67% 23% 6%</div> </div>
1	B	566	<div> <div>10%</div> <div>61% 25% 12%</div> </div>
1	C	566	<div> <div>6%</div> <div>62% 24% 11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	B	1001	-	-	-	X
2	FLC	C	1001	-	-	-	X
3	CL	A	1587	-	-	-	X
3	CL	B	1553	-	-	-	X
4	PGT	A	1588	-	-	-	X
4	PGT	A	1589	-	-	-	X
4	PGT	A	1591	-	-	-	X
4	PGT	B	1554	-	-	-	X
4	PGT	C	1565	-	-	-	X
4	PGT	C	1567	-	-	-	X
5	PEG	B	1555	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12208 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 GLYCINE BETAINES TRANSPORTER BETP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4057	2659	675	707	16			
1	B	497	Total	C	N	O	S	0	0	0
			3742	2473	595	658	16			
1	C	506	Total	C	N	O	S	0	0	0
			3827	2525	613	673	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	GLU	ENGINEERED MUTATION	UNP P54582
A	45	ALA	GLU	ENGINEERED MUTATION	UNP P54582
A	46	ALA	GLU	ENGINEERED MUTATION	UNP P54582
B	44	ALA	GLU	ENGINEERED MUTATION	UNP P54582
B	45	ALA	GLU	ENGINEERED MUTATION	UNP P54582
B	46	ALA	GLU	ENGINEERED MUTATION	UNP P54582
C	44	ALA	GLU	ENGINEERED MUTATION	UNP P54582
C	45	ALA	GLU	ENGINEERED MUTATION	UNP P54582
C	46	ALA	GLU	ENGINEERED MUTATION	UNP P54582

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).

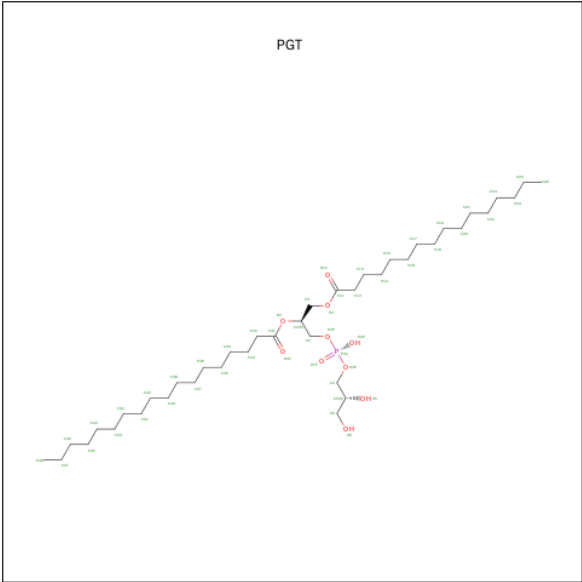


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

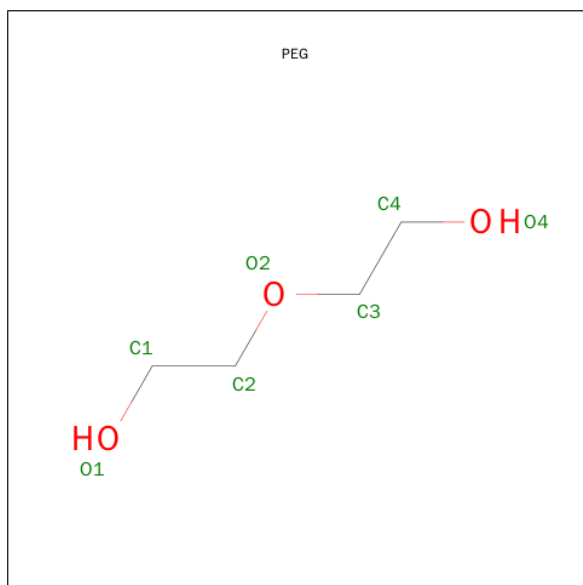
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	C	3	Total	Cl	0	0
			3	3		

- Molecule 4 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C₄₀H₇₉O₁₀P).



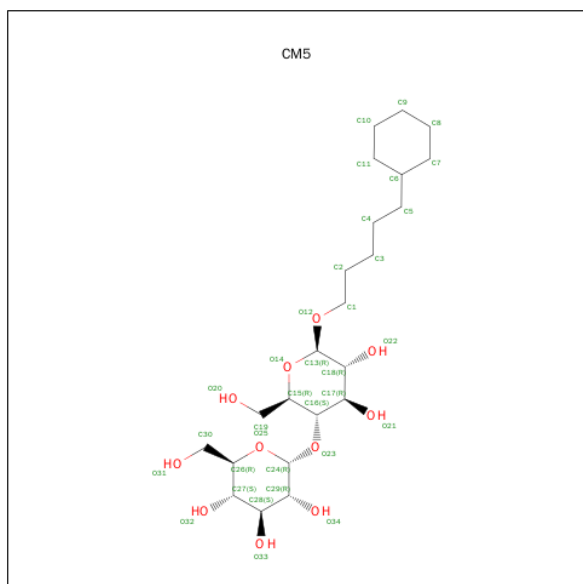
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			51	40	10	1		
4	A	1	Total	C	O	P	0	0
			51	40	10	1		
4	A	1	Total	C	O	P	0	0
			51	40	10	1		
4	A	1	Total	C			0	0
			18	18				
4	A	1	Total	C	O	P	0	0
			51	40	10	1		
4	B	1	Total	C	O	P	0	0
			51	40	10	1		
4	C	1	Total	C	O	P	0	0
			51	40	10	1		
4	C	1	Total	C	O	P	0	0
			51	40	10	1		
4	C	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (three-letter code: CM5) (formula: $C_{23}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			34	23	11		

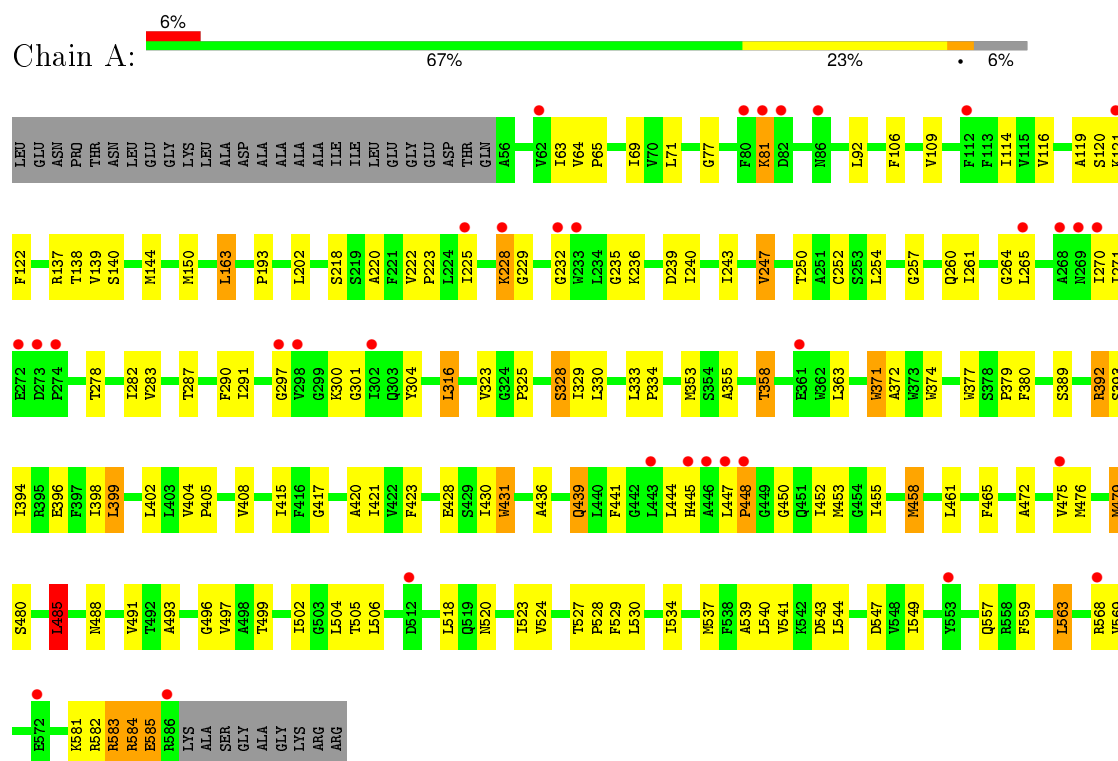
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total 13	O 13	0	0
7	B	23	Total 23	O 23	0	0
7	C	22	Total 22	O 22	0	0

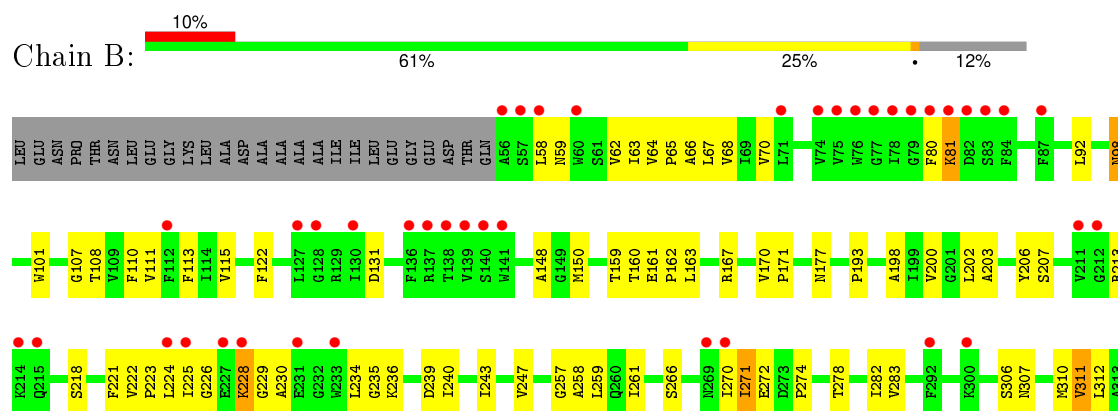
3 Residue-property plots

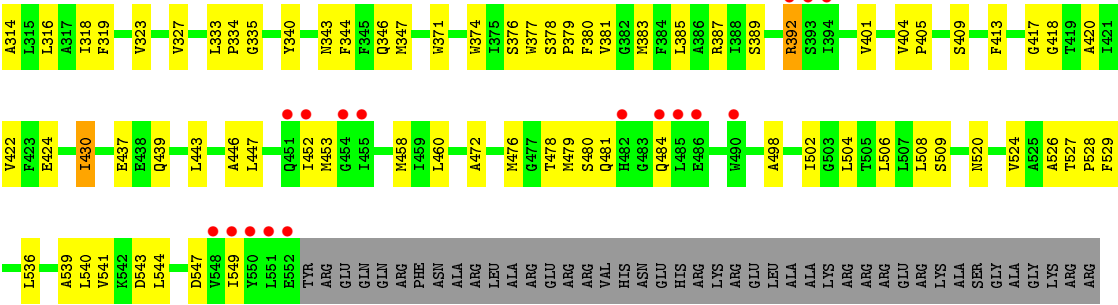
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: GLYCINE BETAINES TRANSPORTER BETP

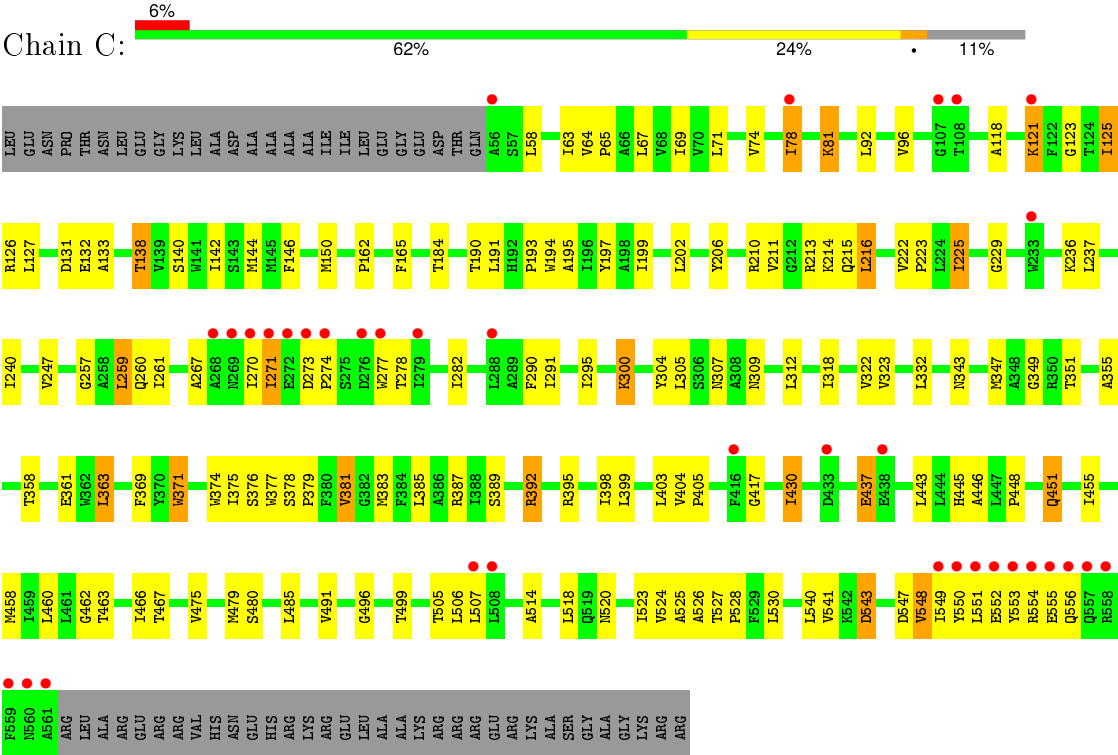


• Molecule 1: GLYCINE BETAINES TRANSPORTER BETP





● Molecule 1: GLYCINE BETAINES TRANSPORTER BETP



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.56Å 129.50Å 167.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.42 – 2.70 47.60 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.42-2.70) 99.7 (47.60-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.212 , 0.266 0.210 , 0.266	Depositor DCC
R_{free} test set	3488 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 83.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 73561 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12208	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PGT, PEG, CM5, FLC, CL

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	0.24	0/4159	0.39	0/5661
1	B	0.24	0/3840	0.40	0/5241
1	C	0.26	0/3927	0.41	0/5357
All	All	0.25	0/11926	0.40	0/16259

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	4057	0	4098	111	0
1	B	3742	0	3775	100	0
1	C	3827	0	3852	118	0
2	A	13	0	5	0	0
2	B	13	0	5	3	0
2	C	26	0	10	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
4	A	222	0	347	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	51	0	78	5	0
4	C	153	0	234	15	0
5	B	7	0	10	0	0
6	C	34	0	42	3	0
7	A	13	0	0	0	0
7	B	23	0	0	2	0
7	C	22	0	0	0	0
All	All	12208	0	12456	352	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 14.

All (352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:CYS:HA	1:A:518:LEU:HD11	1.49	0.92
4:A:1589:PGT:H121	1:C:395:ARG:HD2	1.50	0.90
1:C:81:LYS:HD2	1:C:81:LYS:H	1.49	0.78
1:C:553:TYR:HA	1:C:556:GLN:HG2	1.67	0.76
4:A:1588:PGT:H342	4:A:1592:PGT:H131	1.67	0.76
4:A:1588:PGT:H251	4:A:1591:PGT:H321	1.67	0.75
1:C:312:LEU:HB2	1:C:460:LEU:HD13	1.70	0.72
4:A:1588:PGT:H322	4:A:1588:PGT:H32	1.71	0.72
1:C:547:ASP:OD1	1:C:549:ILE:HG22	1.90	0.72
1:A:430:ILE:O	1:A:431:TRP:HB2	1.89	0.72
1:A:323:VAL:HG11	1:A:448:PRO:HD2	1.70	0.72
4:C:1565:PGT:H431	4:C:1565:PGT:H471	1.72	0.71
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.71	0.71
4:A:1590:PGT:H322	1:C:395:ARG:HG2	1.70	0.71
1:B:259:LEU:HG	1:B:437:GLU:HG2	1.70	0.71
1:A:485:LEU:H	1:A:485:LEU:HD22	1.56	0.71
1:B:161:GLU:HB3	1:B:162:PRO:HD3	1.72	0.70
1:B:163:LEU:HD11	1:B:424:GLU:HG3	1.72	0.69
1:B:430:ILE:HG12	1:B:443:LEU:HA	1.74	0.69
1:C:150:MET:HE1	4:C:1565:PGT:H472	1.76	0.68
1:A:290:PHE:CZ	1:A:496:GLY:HA3	2.28	0.68
1:A:120:SER:HB2	4:A:1589:PGT:H331	1.76	0.67
1:A:330:LEU:HD13	1:B:101:TRP:CE2	2.30	0.66
1:B:225:ILE:HD11	1:B:234:LEU:HD23	1.78	0.66
1:A:92:LEU:HD13	1:A:520:ASN:HA	1.78	0.66
1:A:116:VAL:HG11	4:A:1590:PGT:H221	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:ALA:O	1:C:528:PRO:HD2	1.97	0.65
4:C:1567:PGT:H151	6:C:1568:CM5:H21A	1.77	0.65
1:A:225:ILE:HG23	1:A:229:GLY:HA3	1.79	0.65
4:A:1589:PGT:H322	4:A:1590:PGT:H121	1.78	0.64
1:C:225:ILE:HG23	1:C:229:GLY:HA3	1.78	0.64
1:A:379:PRO:HG3	1:A:529:PHE:CZ	2.32	0.64
1:C:225:ILE:HD11	6:C:1568:CM5:H51	1.77	0.64
4:A:1589:PGT:H221	1:C:191:LEU:HD21	1.80	0.64
1:C:193:PRO:HB3	1:C:374:TRP:CD1	2.33	0.64
1:A:122:PHE:HB3	1:A:544:LEU:HD23	1.80	0.63
4:A:1589:PGT:H5	4:A:1592:PGT:H31	1.80	0.63
1:B:223:PRO:HG3	1:B:543:ASP:OD1	1.98	0.63
1:C:150:MET:O	2:C:1001:FLC:HG1	1.97	0.63
1:A:355:ALA:O	1:A:358:THR:HB	1.97	0.63
1:C:506:LEU:HD23	1:C:518:LEU:HD12	1.80	0.62
1:A:325:PRO:HB2	1:A:328:SER:HB2	1.81	0.62
1:A:452:ILE:HG13	1:A:453:MET:N	2.14	0.62
1:B:306:SER:O	1:B:310:MET:HG2	1.99	0.62
1:A:399:LEU:HD11	4:A:1588:PGT:H182	1.83	0.61
1:A:559:PHE:HE1	1:A:563:LEU:HD12	1.66	0.61
4:A:1589:PGT:H121	1:C:395:ARG:CD	2.27	0.60
1:B:319:PHE:O	1:B:323:VAL:HG22	2.01	0.60
1:B:261:ILE:HG13	1:B:458:MET:HG2	1.83	0.60
1:B:228:LYS:H	1:B:228:LYS:HD3	1.66	0.60
4:A:1589:PGT:H162	1:C:399:LEU:HD21	1.83	0.60
1:B:452:ILE:HD12	1:B:452:ILE:H	1.67	0.59
1:C:64:VAL:HB	1:C:65:PRO:HD3	1.84	0.59
4:A:1590:PGT:C32	1:C:395:ARG:HG2	2.33	0.59
4:A:1588:PGT:H352	4:A:1589:PGT:H392	1.85	0.59
4:C:1565:PGT:H371	4:C:1565:PGT:H471	1.84	0.59
1:A:581:LYS:HG3	1:A:582:ARG:N	2.16	0.59
1:C:383:MET:SD	1:C:475:VAL:HG13	2.43	0.59
1:A:119:ALA:HA	4:A:1588:PGT:H132	1.85	0.59
4:A:1589:PGT:H342	4:A:1589:PGT:H31	1.84	0.59
1:C:150:MET:O	2:C:1001:FLC:HA1	2.03	0.58
1:B:98:ASN:HD22	1:B:98:ASN:N	2.00	0.58
1:C:309:ASN:HD21	1:C:467:THR:HG21	1.68	0.58
1:B:283:VAL:HG21	1:B:504:LEU:HD13	1.85	0.58
4:B:1554:PGT:H241	4:B:1554:PGT:H201	1.85	0.58
1:A:547:ASP:OD2	1:A:549:ILE:HG22	2.04	0.58
1:A:64:VAL:HB	1:A:65:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:O	1:C:467:THR:HG23	2.04	0.57
1:B:376:SER:HB3	1:B:526:ALA:HB2	1.85	0.57
1:C:291:ILE:O	1:C:295:ILE:HG12	2.04	0.57
1:B:404:VAL:HB	1:B:405:PRO:HD3	1.86	0.57
1:C:215:GLN:HE22	1:C:387:ARG:HD2	1.68	0.57
1:C:165:PHE:CE2	1:C:184:THR:HG22	2.39	0.57
1:B:236:LYS:O	1:B:240:ILE:HG13	2.04	0.57
1:A:287:THR:O	1:A:291:ILE:HG13	2.05	0.57
1:C:125:ILE:HG12	1:C:549:ILE:CG2	2.35	0.57
1:A:323:VAL:CG1	1:A:448:PRO:HD2	2.35	0.57
1:A:114:ILE:HG13	1:A:398:ILE:HD13	1.85	0.57
1:B:478:THR:HG23	1:B:484:GLN:O	2.04	0.57
1:A:430:ILE:HG22	1:A:431:TRP:N	2.20	0.56
1:B:202:LEU:HD23	1:B:540:LEU:HD21	1.86	0.56
1:B:150:MET:O	2:B:1001:FLC:HG2	2.05	0.56
1:A:559:PHE:CE1	1:A:563:LEU:HD12	2.40	0.56
1:B:547:ASP:OD2	1:B:549:ILE:HG22	2.04	0.56
1:B:207:SER:O	1:B:213:ARG:HB2	2.05	0.56
1:B:520:ASN:O	1:B:524:VAL:HG23	2.05	0.56
4:A:1592:PGT:H11	4:A:1592:PGT:C32	2.36	0.56
1:B:312:LEU:HB2	1:B:460:LEU:HD13	1.87	0.56
1:C:202:LEU:HD23	1:C:540:LEU:HD21	1.88	0.55
1:B:113:PHE:HA	4:B:1554:PGT:H151	1.88	0.55
1:B:307:ASN:O	1:B:311:VAL:HG12	2.06	0.55
1:A:257:GLY:O	1:A:261:ILE:HG22	2.05	0.55
1:B:319:PHE:CD2	1:B:453:MET:HG3	2.42	0.55
1:A:537:MET:O	1:A:541:VAL:HG23	2.06	0.55
1:C:355:ALA:O	1:C:358:THR:HG22	2.06	0.55
1:C:259:LEU:HD22	1:C:437:GLU:HG2	1.88	0.55
1:B:160:THR:HG23	1:B:439:GLN:HE22	1.71	0.54
1:C:257:GLY:O	1:C:261:ILE:HG22	2.07	0.54
1:B:193:PRO:HB3	1:B:374:TRP:CD1	2.41	0.54
1:A:140:SER:O	1:A:144:MET:HG3	2.08	0.54
1:A:527:THR:HB	1:A:528:PRO:HD3	1.89	0.54
1:A:389:SER:O	1:A:392:ARG:HB2	2.08	0.54
1:C:215:GLN:NE2	1:C:387:ARG:HD2	2.23	0.53
1:A:472:ALA:O	1:A:476:MET:HG3	2.08	0.53
1:A:228:LYS:HD3	1:A:228:LYS:H	1.74	0.53
1:C:381:VAL:O	1:C:385:LEU:HG	2.09	0.53
1:B:198:ALA:HB2	1:B:401:VAL:HG11	1.91	0.53
1:B:228:LYS:N	1:B:228:LYS:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:HG12	1:C:480:SER:HB2	1.90	0.53
1:C:223:PRO:HG3	1:C:543:ASP:OD1	2.09	0.53
1:C:132:GLU:HG3	1:C:133:ALA:H	1.74	0.53
1:C:369:PHE:HA	1:C:523:ILE:HD11	1.89	0.52
1:A:423:PHE:CD2	1:A:430:ILE:HD13	2.45	0.52
1:A:65:PRO:O	1:A:69:ILE:HG12	2.09	0.52
1:C:92:LEU:HG	1:C:520:ASN:CG	2.29	0.52
1:B:333:LEU:HB2	1:B:334:PRO:CD	2.40	0.52
4:A:1589:PGT:H461	4:A:1592:PGT:H261	1.90	0.52
4:C:1567:PGT:C4	4:C:1567:PGT:H12	2.39	0.52
1:B:381:VAL:O	1:B:385:LEU:HG	2.09	0.52
1:C:259:LEU:HD13	1:C:437:GLU:HG2	1.92	0.52
1:B:340:TYR:HH	1:B:344:PHE:HE2	1.56	0.52
1:A:297:GLY:O	1:A:300:LYS:HG2	2.09	0.51
1:A:121:LYS:O	1:A:121:LYS:HD3	2.10	0.51
1:A:333:LEU:HB2	1:A:334:PRO:CD	2.39	0.51
1:C:121:LYS:HB3	1:C:550:TYR:HD2	1.75	0.51
1:B:63:ILE:HG12	1:B:480:SER:HB2	1.93	0.51
1:B:230:ALA:HA	1:B:235:GLY:HA3	1.93	0.51
4:A:1589:PGT:H232	1:C:191:LEU:HD11	1.93	0.51
1:C:549:ILE:O	1:C:552:GLU:HB2	2.10	0.51
1:A:193:PRO:HB3	1:A:374:TRP:CD1	2.46	0.51
1:A:247:VAL:HG23	1:A:499:THR:HA	1.93	0.51
1:A:530:LEU:O	1:A:534:ILE:HG13	2.12	0.50
1:B:148:ALA:O	2:B:1001:FLC:HA1	2.12	0.50
4:A:1589:PGT:C12	1:C:395:ARG:HD2	2.34	0.50
1:C:351:THR:HA	1:C:363:LEU:HD21	1.93	0.50
1:A:106:PHE:HA	1:A:109:VAL:HB	1.93	0.50
1:B:159:THR:HG23	1:B:420:ALA:HB2	1.93	0.50
1:C:451:GLN:NE2	1:C:451:GLN:H	2.09	0.50
1:C:125:ILE:HG22	1:C:126:ARG:N	2.26	0.49
1:B:379:PRO:HG3	1:B:529:PHE:CZ	2.47	0.49
1:A:138:THR:HA	1:A:392:ARG:NH2	2.27	0.49
1:B:70:VAL:HG11	1:B:498:ALA:HB1	1.94	0.49
1:C:278:THR:O	1:C:282:ILE:HG13	2.12	0.49
1:A:430:ILE:HD12	1:A:430:ILE:N	2.28	0.49
1:A:430:ILE:O	1:A:431:TRP:CB	2.56	0.49
1:B:200:VAL:HG21	1:B:378:SER:HB2	1.95	0.49
1:C:273:ASP:OD1	1:C:274:PRO:HD2	2.11	0.49
1:B:62:VAL:HG12	1:B:236:LYS:HB3	1.95	0.49
1:B:270:ILE:O	1:B:271:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASN:O	1:B:62:VAL:HG22	2.12	0.49
1:A:330:LEU:HD13	1:B:101:TRP:NE1	2.28	0.49
1:A:202:LEU:HD23	1:A:540:LEU:HD21	1.93	0.49
1:A:301:GLY:HA2	1:A:304:TYR:CE2	2.48	0.49
1:B:111:VAL:O	1:B:115:VAL:HG13	2.13	0.49
1:A:264:GLY:HA3	1:A:441:PHE:CZ	2.48	0.49
1:C:74:VAL:HA	1:C:505:THR:HG21	1.94	0.49
1:A:431:TRP:HA	1:A:439:GLN:HE21	1.76	0.48
1:A:568:ARG:HD3	1:C:548:VAL:CG2	2.44	0.48
1:C:323:VAL:CG1	1:C:448:PRO:HD2	2.42	0.48
1:B:389:SER:O	1:B:392:ARG:HB2	2.13	0.48
1:B:380:PHE:C	1:B:380:PHE:CD1	2.86	0.48
1:C:290:PHE:CE2	1:C:496:GLY:HA3	2.48	0.48
1:B:257:GLY:O	1:B:261:ILE:HG22	2.13	0.48
1:B:452:ILE:HD12	1:B:452:ILE:N	2.28	0.48
1:C:132:GLU:CG	1:C:133:ALA:N	2.77	0.48
1:C:376:SER:HB3	1:C:526:ALA:HB2	1.94	0.48
1:B:221:PHE:CE1	1:B:536:LEU:HD13	2.49	0.48
1:A:290:PHE:CZ	1:A:493:ALA:HA	2.49	0.48
1:B:98:ASN:N	1:B:98:ASN:ND2	2.62	0.48
1:C:455:ILE:HA	1:C:458:MET:HE2	1.95	0.48
1:B:80:PHE:N	1:B:80:PHE:CD1	2.81	0.48
1:A:163:LEU:HG	1:A:420:ALA:HB1	1.96	0.48
1:A:423:PHE:HD2	1:A:430:ILE:HD13	1.79	0.48
1:C:65:PRO:HB2	1:C:240:ILE:HD13	1.96	0.48
1:B:266:SER:OG	1:B:274:PRO:HD3	2.13	0.48
1:B:278:THR:O	1:B:282:ILE:HG13	2.13	0.48
1:C:375:ILE:HD12	1:C:530:LEU:HA	1.96	0.48
1:A:300:LYS:HG3	1:A:301:GLY:N	2.29	0.48
1:B:170:VAL:HG13	1:B:171:PRO:HD2	1.94	0.48
1:C:430:ILE:HG12	1:C:443:LEU:HA	1.96	0.48
1:C:267:ALA:HB1	1:C:445:HIS:CE1	2.49	0.48
1:C:462:GLY:O	1:C:466:ILE:HG13	2.13	0.48
1:B:409:SER:O	1:B:413:PHE:HD2	1.97	0.48
4:C:1567:PGT:C11	4:C:1567:PGT:H42	2.44	0.47
1:A:444:LEU:O	1:A:450:GLY:HA3	2.14	0.47
1:C:270:ILE:HG22	1:C:270:ILE:O	2.14	0.47
1:B:206:TYR:CE2	1:B:543:ASP:HB3	2.49	0.47
1:C:71:LEU:O	1:C:74:VAL:HG22	2.14	0.47
1:C:118:ALA:O	1:C:395:ARG:HD3	2.13	0.47
1:C:140:SER:O	1:C:144:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1589:PGT:H361	4:A:1589:PGT:H32	1.96	0.47
1:B:150:MET:O	2:B:1001:FLC:HA2	2.13	0.47
1:C:378:SER:OG	1:C:379:PRO:HD3	2.14	0.47
1:A:81:LYS:HD2	1:A:81:LYS:H	1.78	0.47
1:B:527:THR:HB	1:B:528:PRO:HD3	1.97	0.47
1:B:430:ILE:HD11	1:B:446:ALA:HB2	1.97	0.47
1:B:225:ILE:HG23	1:B:229:GLY:HA3	1.95	0.47
1:C:121:LYS:HB3	1:C:550:TYR:CD2	2.50	0.47
1:A:428:GLU:O	1:A:430:ILE:HD12	2.15	0.47
1:A:581:LYS:O	1:A:585:GLU:HB2	2.14	0.47
1:A:278:THR:O	1:A:282:ILE:HG13	2.15	0.47
1:B:218:SER:HB3	1:B:235:GLY:O	2.14	0.47
1:C:150:MET:HB2	1:C:150:MET:HE2	1.80	0.47
1:A:163:LEU:HD13	1:A:431:TRP:HE3	1.80	0.47
1:A:430:ILE:CG2	1:A:431:TRP:N	2.78	0.47
4:C:1566:PGT:H42	4:C:1566:PGT:H32	1.96	0.46
1:B:203:ALA:HA	1:B:540:LEU:HD13	1.97	0.46
1:C:260:GLN:HA	1:C:437:GLU:HB3	1.98	0.46
1:C:190:THR:O	1:C:193:PRO:HD2	2.15	0.46
1:C:527:THR:HB	1:C:528:PRO:HD3	1.97	0.46
1:C:309:ASN:ND2	1:C:467:THR:HG21	2.30	0.46
1:A:261:ILE:HG21	1:A:282:ILE:HG21	1.98	0.46
1:C:404:VAL:HB	1:C:405:PRO:HD3	1.98	0.46
1:B:226:GLY:HA3	1:B:228:LYS:NZ	2.31	0.46
1:A:264:GLY:HA3	1:A:458:MET:HE1	1.98	0.46
1:C:206:TYR:CE2	1:C:210:ARG:HG2	2.51	0.46
1:C:430:ILE:HD12	1:C:430:ILE:HA	1.73	0.46
1:C:138:THR:O	1:C:142:ILE:HG13	2.14	0.46
1:C:304:TYR:O	1:C:307:ASN:HB2	2.16	0.46
4:C:1567:PGT:C35	4:C:1567:PGT:C31	2.94	0.46
1:C:132:GLU:CG	1:C:133:ALA:H	2.29	0.46
1:A:232:GLY:O	1:A:236:LYS:HG2	2.16	0.46
1:A:236:LYS:O	1:A:240:ILE:HG13	2.16	0.46
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.76	0.46
1:A:228:LYS:CD	1:A:228:LYS:H	2.29	0.45
1:B:243:ILE:HG12	1:B:479:MET:HE2	1.98	0.45
1:C:206:TYR:O	1:C:210:ARG:HB3	2.16	0.45
1:B:333:LEU:HB2	1:B:334:PRO:HD2	1.97	0.45
1:C:270:ILE:O	1:C:271:ILE:HG13	2.16	0.45
1:A:353:MET:HE2	1:C:332:LEU:HD21	1.98	0.45
1:A:222:VAL:N	1:A:223:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LYS:HB2	1:C:214:LYS:HZ3	1.82	0.45
1:B:80:PHE:O	1:B:81:LYS:C	2.55	0.45
1:A:63:ILE:HG12	1:A:480:SER:HB2	1.99	0.45
1:B:81:LYS:HG3	1:B:509:SER:HA	1.98	0.45
1:A:380:PHE:HA	1:A:475:VAL:HG11	1.98	0.45
1:A:520:ASN:O	1:A:524:VAL:HG23	2.17	0.45
1:A:254:LEU:HD22	1:A:465:PHE:CE2	2.51	0.45
1:A:493:ALA:O	1:A:497:VAL:HG23	2.17	0.45
1:B:323:VAL:HG23	1:B:447:LEU:HD13	1.99	0.45
1:B:418:GLY:O	1:B:422:VAL:HG23	2.17	0.45
4:A:1592:PGT:H381	4:A:1592:PGT:H412	1.80	0.44
1:C:318:ILE:O	1:C:322:VAL:HG23	2.17	0.44
1:C:138:THR:HA	1:C:392:ARG:HH22	1.83	0.44
1:A:488:ASN:HD22	1:A:491:VAL:HG23	1.82	0.44
1:C:507:LEU:HD23	1:C:514:ALA:HB1	1.99	0.44
1:B:243:ILE:O	1:B:247:VAL:HG23	2.17	0.44
1:B:424:GLU:HG2	7:B:2023:HOH:O	2.17	0.44
1:B:378:SER:OG	1:B:379:PRO:HD3	2.17	0.44
1:A:150:MET:HG2	1:A:408:VAL:HG11	1.98	0.44
1:C:343:ASN:O	1:C:347:MET:HG3	2.17	0.44
1:A:260:GLN:HG2	1:A:461:LEU:HD11	2.00	0.44
1:C:318:ILE:HD11	4:C:1565:PGT:H412	1.98	0.44
1:A:239:ASP:O	1:A:243:ILE:HG13	2.17	0.44
1:C:194:TRP:CE3	1:C:197:TYR:HD2	2.35	0.44
1:C:195:ALA:O	1:C:199:ILE:HG13	2.18	0.44
1:C:236:LYS:HA	1:C:236:LYS:HD3	1.85	0.44
1:A:583:ARG:HA	1:A:583:ARG:HE	1.83	0.44
1:A:584:ARG:H	1:A:584:ARG:CD	2.30	0.44
1:A:243:ILE:O	1:A:247:VAL:HG12	2.18	0.44
1:A:261:ILE:CG2	1:A:282:ILE:HG21	2.47	0.43
1:C:323:VAL:HG11	1:C:448:PRO:HD2	2.00	0.43
1:C:213:ARG:NH2	1:C:543:ASP:OD2	2.50	0.43
1:A:218:SER:HB3	1:A:235:GLY:O	2.18	0.43
1:C:305:LEU:CB	1:C:467:THR:HG22	2.48	0.43
1:B:162:PRO:HG2	1:B:417:GLY:HA3	2.00	0.43
1:C:222:VAL:N	1:C:223:PRO:CD	2.81	0.43
1:A:488:ASN:ND2	1:A:491:VAL:HG23	2.33	0.43
4:B:1554:PGT:H192	4:B:1554:PGT:H222	1.58	0.43
1:A:436:ALA:HA	1:A:439:GLN:OE1	2.18	0.43
1:B:222:VAL:HB	1:B:223:PRO:HD3	1.99	0.43
1:A:371:TRP:CA	1:A:371:TRP:CE3	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD22	1:A:520:ASN:CG	2.39	0.43
1:C:74:VAL:O	1:C:78:ILE:HB	2.19	0.43
1:C:389:SER:O	1:C:392:ARG:HB2	2.19	0.43
1:A:475:VAL:O	1:A:479:MET:HB2	2.19	0.43
1:A:584:ARG:H	1:A:584:ARG:HD3	1.83	0.43
1:C:371:TRP:CE3	1:C:371:TRP:N	2.86	0.43
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.83	0.43
4:A:1589:PGT:H222	1:C:403:LEU:HD21	1.99	0.43
1:B:64:VAL:O	1:B:68:VAL:HG23	2.18	0.43
4:A:1592:PGT:H222	4:B:1554:PGT:H401	2.01	0.43
1:C:125:ILE:HG12	1:C:549:ILE:HG23	2.00	0.43
1:A:202:LEU:HD11	1:A:394:ILE:HG12	2.00	0.43
1:C:371:TRP:HE3	1:C:371:TRP:N	2.15	0.43
1:B:58:LEU:HD23	1:B:481:GLN:HG2	2.00	0.43
1:A:220:ALA:O	1:A:539:ALA:HB1	2.19	0.43
1:C:65:PRO:O	1:C:69:ILE:HG12	2.19	0.43
1:C:162:PRO:CG	1:C:417:GLY:HA3	2.49	0.43
1:C:121:LYS:HD3	1:C:121:LYS:O	2.19	0.43
4:C:1565:PGT:H402	4:C:1565:PGT:H431	1.63	0.42
1:C:92:LEU:O	1:C:96:VAL:HG23	2.18	0.42
1:C:290:PHE:CZ	1:C:496:GLY:HA3	2.54	0.42
1:C:551:LEU:O	1:C:555:GLU:HB2	2.18	0.42
1:C:541:VAL:HG11	4:C:1567:PGT:H411	2.01	0.42
1:B:59:ASN:HD21	1:B:236:LYS:NZ	2.17	0.42
1:B:314:ALA:O	1:B:318:ILE:HD13	2.19	0.42
1:B:115:VAL:HG21	4:B:1554:PGT:H432	2.00	0.42
1:A:502:ILE:O	1:A:506:LEU:HG	2.19	0.42
1:A:290:PHE:CE2	1:A:496:GLY:HA3	2.55	0.42
1:B:239:ASP:O	1:B:243:ILE:HG13	2.19	0.42
1:C:520:ASN:O	1:C:524:VAL:HG23	2.19	0.42
1:B:224:LEU:HD22	1:B:539:ALA:HB2	2.00	0.42
1:C:211:VAL:O	1:C:211:VAL:HG12	2.19	0.42
1:A:329:ILE:HD13	1:A:415:ILE:HA	2.00	0.42
1:B:502:ILE:O	1:B:506:LEU:HD13	2.20	0.42
1:A:333:LEU:HB2	1:A:334:PRO:HD3	2.00	0.42
1:A:404:VAL:HB	1:A:405:PRO:HD3	2.00	0.42
1:B:258:ALA:HA	1:B:261:ILE:CG2	2.50	0.42
1:B:258:ALA:HA	1:B:261:ILE:HG22	2.01	0.42
1:C:300:LYS:C	1:C:300:LYS:HD2	2.39	0.42
1:C:138:THR:HA	1:C:392:ARG:NH2	2.34	0.42
1:B:472:ALA:O	1:B:476:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:HD12	1:C:216:LEU:HA	1.78	0.42
1:A:371:TRP:HA	1:A:371:TRP:CE3	2.55	0.42
1:B:177:ASN:HA	7:B:2008:HOH:O	2.19	0.42
1:A:393:SER:OG	1:A:396:GLU:HB2	2.19	0.42
1:A:250:THR:HB	1:A:499:THR:HG21	2.02	0.41
1:B:107:GLY:HA2	1:B:110:PHE:CD2	2.55	0.41
4:A:1589:PGT:H231	4:A:1589:PGT:H263	1.83	0.41
1:B:335:GLY:HA2	1:C:349:GLY:O	2.20	0.41
1:A:445:HIS:C	1:A:447:LEU:H	2.24	0.41
1:A:77:GLY:HA3	1:A:505:THR:CG2	2.50	0.41
1:A:283:VAL:O	1:A:287:THR:HB	2.20	0.41
4:C:1567:PGT:C6	6:C:1568:CM5:H11	2.51	0.41
1:B:66:ALA:O	1:B:70:VAL:HG23	2.20	0.41
1:A:455:ILE:HA	1:A:458:MET:HG3	2.03	0.41
1:A:372:ALA:HB1	1:A:523:ILE:HA	2.03	0.41
1:A:119:ALA:HA	4:A:1588:PGT:C13	2.51	0.41
1:C:118:ALA:HB2	1:C:398:ILE:HD12	2.02	0.41
1:C:206:TYR:OH	1:C:547:ASP:HB2	2.21	0.41
1:C:123:GLY:HA3	1:C:395:ARG:NH1	2.36	0.41
1:B:504:LEU:O	1:B:508:LEU:HG	2.20	0.41
1:A:163:LEU:HD13	1:A:431:TRP:CE3	2.56	0.41
4:C:1565:PGT:H142	4:C:1565:PGT:H171	1.81	0.41
1:A:371:TRP:CE3	1:A:371:TRP:N	2.89	0.41
1:C:485:LEU:HD22	1:C:485:LEU:H	1.85	0.41
1:A:265:LEU:HD13	1:A:271:ILE:HD12	2.02	0.41
4:C:1565:PGT:H322	4:C:1565:PGT:H2	1.73	0.41
1:B:383:MET:O	1:B:387:ARG:HG3	2.21	0.41
4:A:1588:PGT:H352	4:A:1589:PGT:C39	2.51	0.40
1:B:343:ASN:O	1:B:347:MET:HG3	2.21	0.40
4:C:1565:PGT:H421	4:C:1566:PGT:H481	2.02	0.40
1:C:58:LEU:HD11	1:C:491:VAL:HG21	2.03	0.40
1:B:92:LEU:HD13	1:B:92:LEU:C	2.42	0.40
1:B:122:PHE:CD1	1:B:544:LEU:HB3	2.57	0.40
1:B:430:ILE:O	1:B:430:ILE:HG23	2.22	0.40
1:A:452:ILE:HG13	1:A:453:MET:H	1.87	0.40
1:C:430:ILE:HD11	1:C:446:ALA:HB2	2.02	0.40
1:B:224:LEU:HD13	1:B:539:ALA:HA	2.04	0.40
1:A:417:GLY:O	1:A:421:ILE:HG13	2.21	0.40
1:C:247:VAL:HG23	1:C:499:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	529/566 (94%)	496 (94%)	28 (5%)	5 (1%)	21	49
1	B	495/566 (88%)	458 (92%)	35 (7%)	2 (0%)	39	69
1	C	504/566 (89%)	476 (94%)	26 (5%)	2 (0%)	39	69
All	All	1528/1698 (90%)	1430 (94%)	89 (6%)	9 (1%)	30	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	583	ARG
1	A	431	TRP
1	B	81	LYS
1	A	585	GLU
1	C	131	ASP
1	A	485	LEU
1	B	272	GLU
1	A	448	PRO
1	C	125	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/439 (94%)	388 (94%)	27 (6%)	21	46
1	B	385/439 (88%)	370 (96%)	15 (4%)	39	70
1	C	393/439 (90%)	366 (93%)	27 (7%)	19	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1193/1317 (91%)	1124 (94%)	69 (6%)	25 52

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	81	LYS
1	A	137	ARG
1	A	139	VAL
1	A	163	LEU
1	A	228	LYS
1	A	247	VAL
1	A	270	ILE
1	A	316	LEU
1	A	328	SER
1	A	358	THR
1	A	363	LEU
1	A	371	TRP
1	A	377	TRP
1	A	392	ARG
1	A	399	LEU
1	A	402	LEU
1	A	439	GLN
1	A	458	MET
1	A	479	MET
1	A	485	LEU
1	A	504	LEU
1	A	543	ASP
1	A	557	GLN
1	A	563	LEU
1	A	569	VAL
1	A	584	ARG
1	B	67	LEU
1	B	98	ASN
1	B	108	THR
1	B	131	ASP
1	B	167	ARG
1	B	228	LYS
1	B	271	ILE
1	B	311	VAL
1	B	327	VAL
1	B	346	GLN

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Mol	Chain	Res	Type
1	B	371	TRP
1	B	377	TRP
1	B	392	ARG
1	B	430	ILE
1	B	541	VAL
1	C	67	LEU
1	C	78	ILE
1	C	81	LYS
1	C	121	LYS
1	C	127	LEU
1	C	138	THR
1	C	146	PHE
1	C	216	LEU
1	C	225	ILE
1	C	237	LEU
1	C	259	LEU
1	C	271	ILE
1	C	277	TRP
1	C	300	LYS
1	C	361	GLU
1	C	363	LEU
1	C	371	TRP
1	C	377	TRP
1	C	381	VAL
1	C	392	ARG
1	C	430	ILE
1	C	437	GLU
1	C	451	GLN
1	C	479	MET
1	C	543	ASP
1	C	548	VAL
1	C	554	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	GLN
1	A	445	HIS
1	A	517	ASN
1	A	573	HIS
1	B	59	ASN
1	B	98	ASN

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Mol	Chain	Res	Type
1	B	215	GLN
1	B	303	GLN
1	B	439	GLN
1	B	451	GLN
1	B	488	ASN
1	B	517	ASN
1	C	215	GLN
1	C	481	GLN
1	C	517	ASN
1	C	560	ASN

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 ⓘ

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 for Mogul analysis.

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	FLC	A	1001	-	3,12,12	0.90	0	3,17,17	1.50	1 (33%)
4	PGT	A	1588	-	50,50,50	0.90	2 (4%)	51,56,56	1.08	2 (3%)
4	PGT	A	1589	-	50,50,50	0.94	2 (4%)	51,56,56	0.98	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGT	A	1590	-	50,50,50	0.91	2 (4%)	51,56,56	1.05	3 (5%)
4	PGT	A	1591	-	17,17,50	0.23	0	16,16,56	0.62	0
4	PGT	A	1592	-	50,50,50	0.89	2 (4%)	51,56,56	1.04	2 (3%)
2	FLC	B	1001	-	3,12,12	0.87	0	3,17,17	1.76	2 (66%)
4	PGT	B	1554	-	50,50,50	0.90	2 (4%)	51,56,56	1.00	3 (5%)
5	PEG	B	1555	-	6,6,6	0.45	0	5,5,5	0.27	0
2	FLC	C	1001	-	3,12,12	0.98	0	3,17,17	2.38	2 (66%)
4	PGT	C	1565	-	50,50,50	0.89	2 (4%)	51,56,56	1.07	3 (5%)
4	PGT	C	1566	-	50,50,50	0.90	2 (4%)	51,56,56	1.04	3 (5%)
4	PGT	C	1567	-	50,50,50	0.91	2 (4%)	51,56,56	1.00	3 (5%)
6	CM5	C	1568	-	36,36,36	0.39	0	49,49,49	0.80	1 (2%)
2	FLC	C	1569	-	3,12,12	0.96	0	3,17,17	2.25	2 (66%)

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	FLC	A	1001	-	-	0/6/16/16	0/0/0/0
4	PGT	A	1588	-	-	1/55/55/55	0/0/0/0
4	PGT	A	1589	-	-	0/55/55/55	0/0/0/0
4	PGT	A	1590	-	-	0/55/55/55	0/0/0/0
4	PGT	A	1591	-	-	0/15/15/55	0/0/0/0
4	PGT	A	1592	-	-	0/55/55/55	0/0/0/0
2	FLC	B	1001	-	-	0/6/16/16	0/0/0/0
4	PGT	B	1554	-	-	0/55/55/55	0/0/0/0
5	PEG	B	1555	-	-	0/4/4/4	0/0/0/0
2	FLC	C	1001	-	-	0/6/16/16	0/0/0/0
4	PGT	C	1565	-	-	2/55/55/55	0/0/0/0
4	PGT	C	1566	-	-	1/55/55/55	0/0/0/0
4	PGT	C	1567	-	-	0/55/55/55	0/0/0/0
6	CM5	C	1568	-	-	0/17/65/65	0/3/3/3
2	FLC	C	1569	-	-	0/6/16/16	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1590	PGT	O2-C31	3.78	1.45	1.34
4	C	1565	PGT	O2-C31	3.81	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1592	PGT	O2-C31	3.83	1.45	1.34
4	C	1566	PGT	O2-C31	3.89	1.45	1.34
4	C	1567	PGT	O2-C31	3.95	1.46	1.34
4	B	1554	PGT	O2-C31	3.98	1.46	1.34
4	A	1588	PGT	O2-C31	4.03	1.46	1.34
4	A	1589	PGT	O2-C31	4.07	1.46	1.34
4	A	1588	PGT	O3-C11	4.10	1.45	1.33
4	B	1554	PGT	O3-C11	4.12	1.45	1.33
4	C	1566	PGT	O3-C11	4.12	1.45	1.33
4	C	1565	PGT	O3-C11	4.15	1.45	1.33
4	C	1567	PGT	O3-C11	4.18	1.45	1.33
4	A	1592	PGT	O3-C11	4.21	1.46	1.33
4	A	1590	PGT	O3-C11	4.32	1.46	1.33
4	A	1589	PGT	O3-C11	4.39	1.46	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1590	PGT	C2-O2-C31	-3.60	109.26	117.89
4	C	1565	PGT	C2-O2-C31	-3.56	109.35	117.89
2	C	1001	FLC	CB-CA-CAC	-3.18	109.87	114.96
2	C	1569	FLC	CB-CA-CAC	-2.79	110.50	114.96
2	C	1569	FLC	CB-CG-CGC	-2.71	110.62	114.96
6	C	1568	CM5	C24-O23-C16	-2.71	110.92	118.01
4	C	1566	PGT	C2-O2-C31	-2.66	111.50	117.89
2	C	1001	FLC	CB-CG-CGC	-2.56	110.86	114.96
4	C	1567	PGT	C2-O2-C31	-2.16	112.71	117.89
2	B	1001	FLC	CB-CA-CAC	-2.16	111.51	114.96
2	B	1001	FLC	CB-CG-CGC	-2.11	111.58	114.96
2	A	1001	FLC	CB-CA-CAC	-2.08	111.64	114.96
4	B	1554	PGT	C2-O2-C31	-2.07	112.92	117.89
4	C	1565	PGT	O3-C11-C12	2.23	118.68	111.90
4	C	1566	PGT	O3-C11-C12	2.37	119.11	111.90
4	B	1554	PGT	O3-C11-C12	2.50	119.52	111.90
4	C	1567	PGT	O3-C11-C12	2.66	120.00	111.90
4	A	1588	PGT	O3-C11-C12	2.72	120.20	111.90
4	A	1592	PGT	O3-C11-C12	2.75	120.29	111.90
4	A	1590	PGT	O3-C11-C12	2.85	120.58	111.90
4	A	1589	PGT	O3-C11-C12	2.91	120.75	111.90
4	C	1565	PGT	O2-C31-C32	3.46	119.06	111.53
4	A	1590	PGT	O2-C31-C32	3.58	119.32	111.53
4	A	1589	PGT	O2-C31-C32	3.74	119.65	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1567	PGT	O2-C31-C32	3.81	119.82	111.53
4	A	1592	PGT	O2-C31-C32	3.89	119.98	111.53
4	B	1554	PGT	O2-C31-C32	4.04	120.31	111.53
4	C	1566	PGT	O2-C31-C32	4.24	120.74	111.53
4	A	1588	PGT	O2-C31-C32	4.57	121.46	111.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1588	PGT	C2-O2-C31-C32
4	C	1565	PGT	C2-O2-C31-O31
4	C	1566	PGT	C2-O2-C31-C32
4	C	1565	PGT	C2-O2-C31-C32

There are no ring outliers.

12 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1588	PGT	8	0
4	A	1589	PGT	16	0
4	A	1590	PGT	4	0
4	A	1591	PGT	1	0
4	A	1592	PGT	6	0
2	B	1001	FLC	3	0
4	B	1554	PGT	5	0
2	C	1001	FLC	2	0
4	C	1565	PGT	8	0
4	C	1566	PGT	2	0
4	C	1567	PGT	6	0
6	C	1568	CM5	3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	531/566 (93%)	0.18	33 (6%) 24 23	58, 102, 170, 244	1 (0%)
1	B	497/566 (87%)	0.42	58 (11%) 6 5	48, 104, 176, 248	0
1	C	506/566 (89%)	0.23	35 (6%) 20 18	48, 86, 159, 215	0
All	All	1534/1698 (90%)	0.27	126 (8%) 14 11	48, 98, 170, 248	1 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	550	TYR	9.9
1	C	559	PHE	7.9
1	C	561	ALA	7.8
1	B	549	ILE	7.2
1	C	553	TYR	7.1
1	A	274	PRO	7.1
1	B	81	LYS	7.0
1	B	552	GLU	7.0
1	C	269	ASN	6.5
1	A	273	ASP	6.3
1	B	84	PHE	6.2
1	C	560	ASN	5.7
1	B	548	VAL	5.4
1	C	277	TRP	5.3
1	C	555	GLU	5.2
1	B	490	TRP	5.2
1	B	551	LEU	5.1
1	B	227	GLU	4.9
1	C	550	TYR	4.8
1	C	274	PRO	4.8
1	C	557	GLN	4.6
1	A	82	ASP	4.5
1	B	75	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	486	GLU	4.5
1	A	512	ASP	4.4
1	B	300	LYS	4.4
1	C	556	GLN	4.4
1	B	270	ILE	4.4
1	C	271	ILE	4.3
1	B	228	LYS	4.3
1	B	76	TRP	4.2
1	A	80	PHE	4.2
1	B	485	LEU	4.1
1	B	78	ILE	4.1
1	C	554	ARG	4.1
1	B	56	ALA	3.9
1	B	214	LYS	3.9
1	A	553	TYR	3.8
1	A	586	ARG	3.8
1	B	80	PHE	3.7
1	B	137	ARG	3.7
1	A	233	TRP	3.6
1	C	558	ARG	3.6
1	B	140	SER	3.6
1	B	82	ASP	3.5
1	B	83	SER	3.5
1	B	57	SER	3.5
1	C	270	ILE	3.5
1	A	269	ASN	3.4
1	B	455	ILE	3.4
1	C	551	LEU	3.4
1	A	446	ALA	3.3
1	A	302	ILE	3.3
1	C	288	LEU	3.3
1	B	77	GLY	3.3
1	A	445	HIS	3.3
1	B	224	LEU	3.3
1	B	139	VAL	3.2
1	B	58	LEU	3.2
1	C	272	GLU	3.2
1	C	433	ASP	3.1
1	A	448	PRO	3.1
1	A	447	LEU	3.0
1	A	62	VAL	3.0
1	B	87	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	130	ILE	3.0
1	B	128	GLY	3.0
1	C	56	ALA	3.0
1	B	482	HIS	2.9
1	C	268	ALA	2.9
1	B	292	PHE	2.9
1	B	392	ARG	2.9
1	C	508	LEU	2.9
1	B	138	THR	2.9
1	B	484	GLN	2.8
1	B	60	TRP	2.8
1	B	212	GLY	2.8
1	B	71	LEU	2.7
1	B	394	ILE	2.7
1	A	86	ASN	2.7
1	B	233	TRP	2.7
1	A	443	LEU	2.7
1	A	112	PHE	2.6
1	B	74	VAL	2.6
1	C	279	ILE	2.6
1	C	121	LYS	2.5
1	C	549	ILE	2.5
1	A	270	ILE	2.5
1	B	269	ASN	2.5
1	A	297	GLY	2.4
1	B	211	VAL	2.4
1	C	107	GLY	2.4
1	C	507	LEU	2.4
1	A	265	LEU	2.4
1	A	121	LYS	2.4
1	B	79	GLY	2.3
1	A	268	ALA	2.3
1	B	215	GLN	2.3
1	A	572	GLU	2.3
1	A	232	GLY	2.3
1	B	451	GLN	2.3
1	A	568	ARG	2.3
1	B	452	ILE	2.3
1	A	272	GLU	2.2
1	A	475	VAL	2.2
1	B	127	LEU	2.2
1	A	228	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	438	GLU	2.2
1	B	136	PHE	2.1
1	A	225	ILE	2.1
1	C	78	ILE	2.1
1	A	298	VAL	2.1
1	C	416	PHE	2.1
1	A	361	GLU	2.1
1	C	276	ASP	2.1
1	B	454	GLY	2.1
1	B	225	ILE	2.1
1	B	231	GLU	2.1
1	B	393	SER	2.1
1	C	108	THR	2.0
1	B	112	PHE	2.0
1	B	141	TRP	2.0
1	A	81	LYS	2.0
1	C	552	GLU	2.0
1	C	233	TRP	2.0
1	C	273	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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PGT	A	1591	18/51	0.83	0.77	19.85	86,92,114,114	0
3	CL	A	1587	1/1	0.95	0.36	6.81	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FLC	C	1001	13/13	0.91	0.36	4.58	133,140,145,145	0
4	PGT	A	1588	51/51	0.47	0.46	3.58	85,136,175,236	0
2	FLC	B	1001	13/13	0.74	0.33	3.52	140,150,161,162	0
4	PGT	C	1567	51/51	0.59	0.36	3.25	107,157,233,319	0
4	PGT	A	1589	51/51	0.53	0.49	3.07	74,132,232,385	0
4	PGT	C	1565	51/51	0.66	0.33	2.95	106,176,230,291	0
5	PEG	B	1555	7/7	0.77	0.26	2.09	146,152,153,155	0
4	PGT	C	1566	51/51	0.72	0.20	1.89	109,144,184,223	0
2	FLC	A	1001	13/13	0.85	0.27	1.85	147,163,169,170	0
4	PGT	B	1554	51/51	0.36	0.51	1.85	72,136,208,240	0
6	CM5	C	1568	34/34	0.75	0.29	1.24	112,182,209,211	0
3	CL	B	1553	1/1	0.94	0.48	1.06	109,109,109,109	0
4	PGT	A	1590	51/51	0.76	0.28	1.04	72,99,130,231	0
4	PGT	A	1592	51/51	0.54	0.34	0.63	69,150,203,314	0
3	CL	C	1564	1/1	0.98	0.16	0.13	85,85,85,85	0
3	CL	C	1562	1/1	0.98	0.10	-1.05	74,74,74,74	0
3	CL	C	1563	1/1	0.97	0.09	-1.60	64,64,64,64	0
2	FLC	C	1569	13/13	0.70	0.39	-	188,193,208,210	0

6.5 Other polymers [i](#)

There are no such residues in this entry.